

# Photon diffusion coefficient in an absorbing medium

Raphael Aronson

NIR<sub>x</sub> Medical Technologies, West Orange, New Jersey 07052

Noel Corngold

California Institute of Technology, Pasadena, California 91125

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A number of investigators have recently claimed, based on both analysis from transport theory and transport-theory-based Monte Carlo calculations, that the diffusion coefficient for photon migration should be taken to be independent of absorption. We show that these analyses are flawed and that the correct way of extracting diffusion theory from transport theory gives an absorption-dependent diffusion coefficient. Experiments by two different sets of investigators give conflicting results concerning whether the diffusion coefficient depends on absorption. The discrepancy between theory and the earlier set of experiments poses an interesting challenge. © 1999 Optical Society of America [S0740-3232(99)02205-X]

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## 1. INTRODUCTION

In the past few years there has been much interest in photon migration in tissue.<sup>1-3</sup> It has been generally accepted that transport theory serves as a good model for this migration. In practice, however, the extreme optical thickness and complexity of body organs have led investigators to use diffusion theory, which is generally more computationally tractable. The diffusion equation involves two medium-dependent parameters, the diffusion coefficient  $D$  and the absorption coefficient  $\mu_a$ , and it is important that these be chosen correctly.

Recent experiments by Bassani *et al.*<sup>4</sup> give results that can be understood nicely in terms of a simple version of diffusion theory, in which the diffusion coefficient is taken to be independent of absorption. This result would appear to be satisfying because several authors, proceeding from a mathematical analysis of the transport equation, have claimed to derive that independence.<sup>5-8</sup> It is our purpose here to show that those analyses are flawed and that a proper derivation of diffusion theory from transport theory predicts a dependence of the diffusion coefficient on absorption. Thus these experiments, rather than supporting a simple theory, indicate a discrepancy that requires explanation. (By contrast, very recently, after the submission of this paper, experimental results have been published by Rinzema *et al.*<sup>9</sup> that support our conclusions. See *Note added in proof* below, just preceding the References. This is the later set of experiments referred to in the abstract.)

The reasoning by which these papers arrive at their conclusion is threefold:

1. Experimental: This is the result of varying the absorption in various media, measuring the intensity over some range, and fitting the result to the best diffusion coefficient.<sup>4</sup>

2. Analytical: This is what transport theory gives when looked at correctly.<sup>5-7</sup>

3. Numerical: This is what time-dependent Monte Carlo calculations give.<sup>4,7,8</sup>

By contrast, we assert that

1. Transport theory says that the diffusion coefficient does depend on the absorption.

2. It is the time-independent rather than the time-dependent equation that should be examined to obtain the diffusion coefficient.

3. Monte Carlo calculations (especially time-dependent Monte Carlo) are both overkill and underkill. They give, with substantial error and with the expenditure of considerable computer time and effort, results that can be computed exactly to a large number of significant figures in small fractions of a second on any reasonable desktop computer.

We have calculated  $D$  by transport theory for a number of different absorption strengths and phase functions, and we find apparent disagreement with the experimental results of Bassani *et al.*<sup>4</sup> We discuss below some possible reasons for the discrepancies, but in the end we are not able to resolve them.

## 2. ANALYSIS

The transport equation is a continuity equation that enforces a particle balance in each element of volume and solid angle (and time, for the time-dependent version). It assumes that the collisions are or can be approximated by point collisions in both space and time. When applied to light, it assumes also that a photon picture is valid, i.e., that the light is incoherent. The time-independent and time-dependent transport equations for a homogeneous

medium in which the only processes allowed are elastic scattering and absorption (well justified in our context) are given, respectively, by

$$\hat{\Omega} \cdot \nabla I(\mathbf{r}, \hat{\Omega}) + \mu_t I(\mathbf{r}, \hat{\Omega}) = \mu_s \int p(\hat{\Omega} \cdot \hat{\Omega}') I(\mathbf{r}, \hat{\Omega}') d\hat{\Omega}' + S(\mathbf{r}, \hat{\Omega}) \quad (1)$$

and

$$\frac{1}{c} \frac{\partial I(\mathbf{r}, \hat{\Omega}, t)}{\partial t} + \hat{\Omega} \cdot \nabla I(\mathbf{r}, \hat{\Omega}, t) + \mu_t I(\mathbf{r}, \hat{\Omega}, t) = \mu_s \int p(\hat{\Omega} \cdot \hat{\Omega}') I(\mathbf{r}, \hat{\Omega}', t) d\hat{\Omega}' + S(\mathbf{r}, \hat{\Omega}, t). \quad (2)$$

Here  $\mathbf{r}$  is the position variable,  $\hat{\Omega}$  a unit vector in the direction of particle motion, and  $t$  the time. The medium-dependent parameters are the total attenuation coefficient  $\mu_t$ ; the scattering coefficient  $\mu_s$ ; the phase function  $p(\hat{\Omega} \cdot \hat{\Omega}')$  for scattering from direction  $\hat{\Omega}'$  to direction  $\hat{\Omega}$ , normalized so that its integral over all solid angle is unity; and the speed  $c$  of light in the medium.  $I(\mathbf{r}, \hat{\Omega}, t)$  is the angular intensity at  $\mathbf{r}$ ,  $\hat{\Omega}$ , and  $t$  per unit solid angle; and  $S(\mathbf{r}, \hat{\Omega}, t)$  is the source strength at  $\mathbf{r}$ ,  $\hat{\Omega}$ , and  $t$  per unit volume, time, and solid angle. Equation (1) is just a steady-state version of Eq. (2). The absorption coefficient is given by  $\mu_a = \mu_t - \mu_s$ .

For future reference, we note the spherical harmonic expansion of the phase function:

$$p(x) = \sum_{l=0}^L \frac{2l+1}{4\pi} f_l P_l(x), \quad (3)$$

where the sum may be cut off at some finite value  $l = L$ . The normalization is such that  $f_0 = 1$ . The quantity  $f_1$ , which is the average value of the cosine of the scattering angle, is sometimes called the anisotropy parameter and given the alternate symbol  $g$ . For Henyey-Greenstein scattering,  $f_l = g^l$ .

The solution of the transport equation is controlled by the system parameters defined above, the source strength, the boundary conditions, and, for the time-dependent problem, the distribution of particles at  $t = 0$ . A typical diffusion equation may be regarded as an approximation to the transport equation. One may derive different diffusion equations from Eq. (1) or Eq. (2) with different approaches. In general the key diffusion parameter  $D$  is a functional of  $\mu_s$ ,  $\mu_a$ , and the partial-wave expansion coefficients  $f_l$ .

### A. $P_1$ Analysis

The analysis in Refs. 5–8 goes from Eq. (2) to diffusion theory by means of the so-called  $P_1$  approximation, in which the transport equation is expanded in spherical harmonics and only the  $l = 0$  and  $l = 1$  (isotropic and linearly anisotropic) terms are retained in the angular expansion of the intensity. In addition, one neglects any anisotropy in the source. The result is the pair of coupled equations

$$\frac{1}{c} \frac{\partial \phi(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{J}(\mathbf{r}, t) + \mu_a \phi(\mathbf{r}, t) = S(\mathbf{r}, t), \quad (4)$$

$$\frac{1}{c} \frac{\partial \mathbf{J}(\mathbf{r}, t)}{\partial t} + \frac{1}{3} \nabla \phi(\mathbf{r}, t) + \mu_{tr} \mathbf{J}(\mathbf{r}, t) = 0. \quad (5)$$

Here  $\phi(\mathbf{r}, t)$  is the intensity and  $\mathbf{J}(\mathbf{r}, t)$  the flux at  $(\mathbf{r}, t)$ , and  $\mu_{tr}$  is the transport cross section, defined by

$$\mu_{tr} = (1 - g)\mu_s + \mu_a \equiv \mu_{s'} + \mu_a, \quad (6)$$

where  $\mu_{s'}$  is sometimes called the reduced scattering coefficient.

Equation (4) is just a continuity equation, as is the transport equation, and it is exact. The telegrapher's equation is obtained by eliminating  $\mathbf{J}$  between these two equations. The diffusion equation results from first dropping the time-derivative term in Eq. (5). The resulting relation is Fick's law, which when inserted into Eq. (4) to eliminate  $\mathbf{J}$  produces the diffusion equation

$$\frac{1}{c} \frac{\partial \phi(\mathbf{r}, t)}{\partial t} - D \nabla^2 \phi(\mathbf{r}, t) + \mu_a \phi(\mathbf{r}, t) = S(\mathbf{r}, t), \quad (7)$$

where  $D$  is given by

$$D = 1/3\mu_{tr}. \quad (8)$$

For a given set of boundary conditions and initial distribution, the solutions of both the source-free version of the time-dependent transport equation, Eq. (2), and the  $P_1$  approximation to it, Eqs. (4) and (5), depend on  $\mu_a$  according to the relation

$$f(\mu_a) = f(\mu_a = 0) \exp(-\mu_a c t). \quad (9)$$

Furutsu and Yamada<sup>5,6</sup> and Durduran *et al.* in their earlier paper<sup>7</sup> assert that for a pulse source, Eq. (9) should hold for the solution of the time-dependent diffusion equation as well. Inspection of Eq. (7) shows immediately that this is equivalent to requiring that  $D$  be independent of  $\mu_a$ . From this they conclude that one should use Eq. (8) for the case in which  $\mu_{tr}$  is given its value for  $\mu_a = 0$ ; i.e.,

$$D = 1/3\mu_{s'}. \quad (10)$$

This is an erroneous conclusion, on two grounds. First, Eq. (9) does not survive the transition to the diffusion equation at all. Neglecting the time-derivative term in Eq. (5) destroys Eq. (9); the  $\mu_a$  part of  $\mu_{tr}$  in Eq. (5) can no longer be removed by applying Eq. (9). None of the cited papers<sup>5–8</sup> prove that Eq. (9) holds for the solution of the diffusion equation; they merely assert it. The assertion is false, and therefore it is not true that transport theory predicts in any guise or approximation that  $D$  is independent of absorption. In their later paper<sup>8</sup> Durduran *et al.* recognize this but remain neutral on what  $D$  should be, finally deciding to leave the decision to the results of a Monte Carlo calculation.

Second, even if Eq. (9) were correct, it does not imply Eq. (10) as a logical consequence. There is no logical reason for preferring  $D = 1/3\mu_{s'}$  to  $D = 1/3(\mu_{s'} + \mu_{a0})$ , where  $\mu_{a0}$  can assume any value whatever.

This argument can be put in another way. Substituting  $\phi = \psi \exp(-\mu_a ct)$  into Eq. (7) eliminates the absorption term (the one with  $\mu_a$ ) but does not change any original dependence of  $D$  on  $\mu_a$ .

### B. Other Derivations of Diffusion Theory

Diffusion theory is extremely robust, in that it is the lowest-order approximation to transport theory almost no matter how the approximation is made. Some well-known approaches, all assuming isotropic scattering, are a random-walk or random-flight approach,<sup>10</sup> elementary kinetic theory,<sup>11</sup> and a consistent asymptotic scaling.<sup>12</sup> They do not necessarily all lead to the same expression for  $D$ . For instance, the kinetic theory approach gives neither Eq. (8) nor Eq. (10) but<sup>11</sup>  $D = \mu_s/3\mu_t$ . All the expressions for  $D$  are, however, the same to first order in  $\mu_a/\mu_t$ .

All of these approaches require that  $\mu_a \ll \mu$ . Contrary to the assertions of Furutsu and Yamada,<sup>5,6</sup> the  $P_1$  approximation requires this as well. Physically this is because it assumes a nearly isotropic intensity distribution, implying that the flux is small, which in turn by Fick's law implies a small intensity gradient, something incompatible with large absorption. It is for this reason that the question of precisely which value to use for the diffusion coefficient has been of little concern up to now. It is only with recent work on migration of infrared radiation in tissue that the issue has arisen, because the media of interest may be extremely thick, and small differences in  $D$  can make large differences in the solutions deep in the medium.

### C. Diffusion Theory in the Asymptotic Region

There is one regime in which diffusion theory is valid and the absorption need not be small, and that is in the asymptotic region, at many mean free paths from strong sources and boundaries and at late times compared with the mean free time. (This is not asymptotic in the sense of the work of Larsen and Keller,<sup>12</sup> which requires that there be some parameter of smallness in which a consistent expansion of the transport equation can be made.)

Consider first the sourceless time-independent transport equation in a half-space. The analysis given by Case and Zweifel<sup>13</sup> shows that the solution is made up of a transient component that becomes negligible several mean free paths from the boundary, plus one or more terms, each of which falls off exponentially with an attenuation length larger than a mean free path. For isotropic or linearly anisotropic scattering, there is only one of these exponential terms; as the scattering becomes strongly anisotropic, more of these terms can appear.<sup>14,15</sup> At a distance from the boundary sufficiently large that only the dominant term remains, the solution is exponential and therefore satisfies the diffusion equation in this asymptotic region. This exponential attenuation length  $\nu$  is the desired diffusion length and is to be identified with  $\sqrt{D/\mu_a}$ , since that is the attenuation length predicted by Eq. (7). Once  $\nu$  is determined for a given value of  $\mu_a$ , this suffices to calculate  $D$ . In their classic monograph of nearly half a century ago, Case *et al.*<sup>16</sup> define  $D$  in this way. We argue that this is the proper definition, and we have used it to calculate  $D$ . This is in fact the

regime in which both the Monte Carlo calculations<sup>4,8</sup> and the experiments<sup>4</sup> to which we refer were done. We stress that this and only this diffusion solution is the correct solution of the transport equation in the bulk of the medium.

Case *et al.*<sup>16</sup> give the dispersion relation that determines  $\nu$  for isotropic scattering. The equation, quoted by Case and Zweifel,<sup>13</sup> is

$$\frac{\varpi \nu}{2} \ln \frac{\nu + 1}{\nu - 1} = 1, \quad (11)$$

where  $\varpi = \mu_s/\mu_t$  and  $\nu$  is given in units of the mean free path. Even though a numerical computation is easy, it is still instructive to examine the analytical solution of Case *et al.*,<sup>16</sup> which is given in the form of an expansion in  $1 - \varpi = \mu_a/\mu_t$ . This is easily obtained from Eq. (11) by successive approximations. The result is<sup>16</sup>

$$\begin{aligned} 1/\nu^2 = 3(1 - \varpi) & \left[ 1 - \frac{4}{5}(1 - \varpi) + \frac{4}{175}(1 - \varpi)^2 \right. \\ & + \frac{4}{175}(1 - \varpi)^3 + \frac{7556}{336,875}(1 - \varpi)^4 \\ & \left. + \frac{471,844}{21,896,875}(1 - \varpi)^5 + \dots \right], \quad (12) \end{aligned}$$

from which  $1/D = 3\mu_t$  times the quantity in the brackets. (For isotropic scattering,  $\mu_{tr} = \mu_t$ .) Replacing the factor in the bracket by unity for small  $\varpi$  gives Eq. (8). However, that is not an appropriate procedure, since it neglects terms in  $\mu_a/\mu_t$  of the same order as the one retained. The correct result to first order in the absorption is

$$1/D = 3\mu_t \left( 1 - \frac{4}{5} \frac{\mu_a}{\mu_t} \right) = 3(\mu_s + 0.2\mu_a). \quad (13)$$

This is closer numerically to Eq. (10) than to Eq. (8). However, it does not say that the absorption can be neglected altogether.

Holte<sup>17,18</sup> has derived a more general expansion formula valid for anisotropic scattering, to wit:

$$\begin{aligned} \frac{1}{\nu^2} = h_0 h_1 & \left[ 1 - \frac{4h_0}{h_2} + \left( \frac{4h_0}{h_2} \right)^2 \left( 1 - \frac{9h_1}{4h_3} \right) - \left( \frac{4h_0}{h_2} \right)^3 \right. \\ & \left. \times \left( 1 - \frac{27h_1}{4h_3} + \frac{81h_1^2}{16h_3^2} + 9 \frac{h_1^2 h_2}{h_3^2 h_4} \right) + \dots \right], \quad (14) \end{aligned}$$

where

$$h_l = (2l + 1)(1 - \varpi f_l), \quad (15)$$

and the  $f_l$  are defined by Eq. (3). Then  $f_1 = g$ ,  $h_0 = \mu_a/\mu_t$ ,  $h_1 = 3\mu_{tr}/\mu_t$ , and  $1/D = 3\mu_{tr}$  times the quantity in brackets. Again, consistency requires that at least the first-order term in the brackets be taken into account. Equation (14) reduces to Eq. (12) when  $f_l = 0$ ,  $l > 0$ , but does not in general lead to a neat form for the diffusion coefficient such as Eq. (13). It is less accurate than Eq. (12) because the quantity in the brackets goes only to third order in  $h_0$ , two orders less than in Eq. (12). Both Eqs. (12) and (14) are accurate to approximately 1

part in  $10^5$  for  $\varpi > 0.9$  and to approximately 1% for  $\varpi = 0.5$ . In any case, one can calculate  $D$  numerically by using a  $P_N$  approximation,<sup>13</sup> a double- $P_N$  approximation<sup>13</sup> (as we did), or a Chandrasekhar discrete-ordinate approximation,<sup>19</sup> among others, to solve the eigenvalue equation and by increasing the degree of approximation to get as accurate an answer for  $1/D$  as desired.

We remark in passing that the method described by Case and Zweifel gives not only the attenuation length but also the shape of the angular intensity.<sup>13</sup> For isotropic scattering in slab geometry, the distribution is proportional to  $(\nu - \mu)^{-1}$ , where  $\mu$  is the cosine of the angle with the slab normal. When the absorption is small,  $\nu \gg 1$ , so this expression is almost constant and the distribution is almost isotropic; the  $P_1$  approximation is valid. As the absorption increases,  $\nu$  decreases until it becomes unity for 100% absorption, and the distribution can become very anisotropic indeed. This is one way to see why the  $P_1$  approximation fails for large absorption. When the scattering is anisotropic, the distribution is a polynomial in  $\mu$  plus a term proportional to  $(\nu - \mu)^{-1}$ , and one reaches the same conclusion.

#### D. Asymptotic Solutions for Time-Dependent Transport

We asserted in the Introduction that one should examine the time-independent rather than the time-dependent equation to get a value for  $D$ . In this section we discuss the reasons for this assertion.

Bowden<sup>20</sup> has discussed the eigenvalue problem for the time-dependent transport equation for isotropic scattering. Carrying out the procedure leading to Eq. (11) on the Laplace time-transformed equation leads to the dispersion relation

$$\frac{\varpi \kappa}{2(1 + s/c)} \ln \frac{\kappa + 1}{\kappa - 1} = 1, \quad (16)$$

where  $s$  is the Laplace transform variable and

$$\kappa = (1 + s/c)\nu. \quad (17)$$

(Note that our notation differs slightly here from that in Ref. 20, in which the particle speed  $c$  was taken as unity and  $s - 1$  rather than  $s$  was taken as the transform variable.) This equation is identical to Eq. (11) with  $\varpi \rightarrow \varpi/(1 + s/c)$  and  $\nu \rightarrow \kappa$ . Thus one immediately has a solution for which  $\nu$  depends on  $s$ . It follows that the time-dependent solution, which is obtained by Laplace-inverting the solution of the transform equation, has a simple exponential spatial dependence only at long times, to which only the  $s = 0$  transform solution contributes. It follows in turn that the attenuation length of the diffusion mode for the time-dependent equation is identical to that for the static equation, discussed above. The reasoning is the same for anisotropic scattering.

Looking directly at  $D$  perhaps puts the contradiction between an absorption-independent diffusion coefficient for the time-dependent diffusion equation and the exact result of Case *et al.*<sup>16</sup> in perhaps its starkest form. It is obvious (and is also well known) that the solution of the time-independent diffusion equation is obtained from that of the time-dependent equation by integrating over all time. That means that whatever the diffusion coefficient

be for the time-dependent equation, the time-independent equation must have the same  $D$ . But in a time-independent situation we know the result of Case *et al.*<sup>16</sup> to be correct.

We conclude that Monte Carlo calculations for the time-dependent situation must, if they are correct, give the diffusion coefficient valid for the static case, which, as we have pointed out, can be obtained numerically by computationally fast standard methods.

### 3. NUMERICAL RESULTS

The quantity  $\nu$  (or  $\nu^2$ ) can be calculated by standard procedures, either as the largest eigenvalue of a certain eigenvalue equation or, equivalently, from a dispersion relation.<sup>13</sup> We have calculated  $\nu^2$ , and from it  $D$ , by the transfer matrix method<sup>21</sup> in both double- $P_{20}$  and double- $P_{99}$  approximations. A double- $P_{20}$  calculation (a 42-term expansion of the angular intensity) for a single medium takes  $\sim 0.02$  s on a 166-MHz Pentium computer, almost independent of the number of terms in the partial-wave expansion, and it gives six-figure accuracy in  $\nu$  almost down to  $\mu_a/\mu_t = 0.1$ . A double- $P_{99}$  calculation (a 200-term expansion) takes  $\sim 1/3$  s. Note that one does not need to solve a transport problem for the intensity to obtain  $D$ . Geometry is in no way involved, since  $D$  depends only on the properties of the medium.

Since the question addressed here is how the absorption affects the diffusion coefficient, it is convenient to write  $D$  in terms of parameter  $\alpha$  as

$$D = \frac{1}{3(\mu_s' + \alpha\mu_a)}. \quad (18)$$

The point is that the parameter  $\alpha$  should vary much more weakly with absorption than  $D$ . Equation (8) is a special case of this equation with  $\alpha = 1$ , and Eq. (10) is a special case with  $\alpha = 0$ . We have already seen that transport theory predicts  $\alpha = 0.2$  for isotropic scattering and very small absorption. More generally, for small absorption the Holte formula gives  $\alpha = 1 - (4/5)(1 - f_1)/(1 - f_2)$ . We did calculations for Henyey-Greenstein scattering<sup>22</sup> for values of  $\varpi$  from unity down to 0.1 and values of  $g$  up to 0.8. Sample results are given in Table 1. For various values of  $\varpi$  and  $g$  we have tabulated  $D$ ,  $\alpha$ ,  $\nu$ , and  $\nu_2$ , the attenuation length of the second-most-rapidly-attenuated mode. The significance of  $\nu_2$  is that diffusion does not set in until this mode is negligibly small, a few times the distance  $\nu_2$  into the medium. The lengths  $D$ ,  $\nu$ , and  $\nu_2$  are given in units of the mean free path  $\lambda_t = 1/\mu_t$ . All the results are accurate to the precision shown.

Although  $\alpha$  does not vary strongly with absorption, it is a much stronger function of the  $f_l$ . For isotropic or weakly anisotropic ( $g \leq 0.2$ ) scattering it increases somewhat with increasing absorption. For isotropic scattering it is 0.20 or 0.21 for up to 30% absorption, then increases sharply to 0.30 at 90% absorption. For weakly anisotropic scattering the variation is much weaker. For  $g \geq 0.30$ ,  $\alpha$  decreases with increasing absorption. The smallest value we found for  $\alpha$  was 0.20. As can be seen,  $\alpha$  becomes greater than 0.5 for  $g = 0.8$  and absorption probability less than 0.2.

**Table 1. Diffusion Coefficient  $D$ ; Parameter  $\alpha$  Defined by Eq. (18); Diffusion Attenuation Length  $\nu$ ; and Attenuation Length  $\nu_2$  of Transient Modes for Henyey–Greenstein Scattering, All As Functions of Single-Scattering Probability  $\varpi$  and Anisotropy Parameter  $g$**

$\varpi$	$g$	$D$	$\alpha$	$\nu$	$\nu_2$
0.9	0.0	0.362219	0.20	1.90	1.00
0.8	0.0	0.396287	0.21	1.41	1.00
0.5	0.0	0.545367	0.22	1.04	1.00
0.9	0.2	0.442572	0.33	2.10	1.00
0.8	0.2	0.472148	0.33	1.54	1.00
0.5	0.2	0.593280	0.32	1.09	1.00
0.9	0.8	1.435385	0.52	3.79	1.45
0.8	0.8	1.285539	0.50	2.54	1.32

It should be noted that  $\nu_2$  is significantly different from unity only for very anisotropic scattering in which a large number of nonzero  $f_l$  are present. But even the largest value shown in the table,  $1.45 \lambda_t$ , is only about  $\sim 0.4$  transport mean free path, so in practice the boundary region, in which the asymptotic regime is not yet established, is quite small.

#### 4. DISCUSSION OF THE EXPERIMENTAL APPROACH

Bassani *et al.*<sup>4</sup> measured the attenuation length  $\nu$  of photons in a water suspension of either polystyrene spheres or Liposyne 10%, with India ink added as an absorber. Their experiments indicate that  $\nu$  is proportional to the inverse square root of the absorption coefficient. They show that  $D$  from Eq. (10) agrees well with their results to within the error bars, while that from Eq. (8) lies well outside the error bars. The experiments were performed in the asymptotic region, both in space and in time.

Two questions immediately spring to mind: Do the conditions of the experiments satisfy the assumptions of transport theory, and what value of  $D$  does the transport calculation give for the media in which the experiments were performed? We have a partial answer to these questions for the polystyrene spheres but not for the Liposyne.

The radius of the polystyrene spheres was  $r = 0.3995 \mu\text{m}$ ,  $\mu_s' = 1.25 \text{ mm}^{-1}$ ,  $g = 0.898$ , and the ratio of the scattering cross section to the geometrical cross section was  $\gamma = 1.885$ . The first two numbers are given in the paper of Bassani *et al.*<sup>4</sup> and the last two were kindly communicated to us by Giovanni Zaccanti.<sup>23</sup> Since  $\mu_s' = (1 - g)N\gamma\pi r^2$ , where  $N$  is the density of spheres, these numbers give  $N = 1.3 \times 10^{10} \text{ spheres cm}^{-3}$ , from which the mean spacing between spheres is  $a = N^{1/3} = 4 \mu\text{m}$ . This is large compared with both the wavelength of the light used (634 nm) and the particle diameter, and it is small compared to the mean free path. Under these conditions, transport theory should apply. Unfortunately, no comparable estimates are available for the Liposyne spheres, so it is not clear whether one should expect transport theory to hold for those experiments.

Presumably the polystyrene spheres are Mie scatterers, and their diameters are quite uniform. If the partial-wave coefficients of the Mie scattering were available, one could compute  $\alpha$  and  $D$ . They are not available at present, but we hope that they will be in the near future. It may be that the results will be consistent with the experiments. They will certainly be intermediate between those of the two models that Bassani *et al.*<sup>4</sup> considered.

Theory and experiment will be harder to bring into harmony for the Liposyne spheres. We have no information about the size and density of scatterers, and we know little about the phase function and the scattering cross section. Perhaps more important, the error bars on the experiments seem to show little leeway for any value of  $\alpha$  much different from zero. Thus even if we could determine that the experiments are in the regime in which transport theory holds and if we could actually obtain the input data with which to calculate  $\nu^2$ , it does not seem likely that the calculated  $\nu^2$  would agree with the experiment.

#### 5. CONCLUSION

There are two issues involved here. One is the relation of diffusion theory to transport theory; the other is the relation between a transport calculation and experiment. We have argued that the proper derivation of diffusion theory from transport theory is the asymptotic approach, in which the diffusion solution is taken to be the dominant discrete mode of the full solution. This is so both because the asymptotic region is the only one in which the intensity curve obtained from transport theory is known to satisfy the diffusion equation and because this is truly the regime of experimental interest in the context of diffusion tomography, the field in which the question of the proper  $D$  to use arose. The asymptotic region may be analyzed whatever the strength of the absorption in the medium or the degree of anisotropy of the photon distribution. One obtains a distinct dependence of diffusion coefficient on absorption. Since this contradicts results obtained by some workers, we have indicated the errors in the arguments that have led others to conclude that no dependence exists.

If the medium satisfies the assumptions of transport theory, agreement with the asymptotic transport theory results is mandatory. The theory unambiguously gives a value of  $D$  that depends on absorption. If the experimental results are correct, any disagreement with the calculations implies that either the medium does not satisfy the assumptions of transport theory or else that the medium is different from that assumed in the calculations. As discussed above, the suspension of polystyrene spheres in the experiments of Bassani *et al.*<sup>4</sup> seems to satisfy the assumptions of transport theory; we do not know whether the Liposyne suspension does. In neither case do we know the values of  $\varpi$  or the  $f_l$ , so no direct comparison of theory with experiment has been made. In view of those results that we have obtained, it seems unlikely that there is any medium in which  $D$  is independent of absorption. If there is, it is a special case; no such result is true in general. It still remains, however, to do a calculation

for the specific media of Bassani *et al.*<sup>4</sup> and make a direct comparison between theory and experiment.

*Note added in proof.* Two papers have appeared recently that support our conclusions. Durian<sup>24</sup> has performed Monte Carlo calculations that he compares with solutions of the telegrapher's equation. He, too, concludes that  $D$  depends on absorption, and recommends  $\alpha = 1/3$ .

Rinzema *et al.*<sup>9</sup> measured the intensity for a point isotropic source in two different media consisting of suspensions of latex spheres in water with a dye added for absorption. In addition, they carried out transport calculations and found excellent agreement with the experimental results. They also tabulated values of  $\kappa_0 = \mu_t/\nu$ . Using their published  $\mu_s$ ,  $\mu_a$  and  $g$ , plus the appropriate values of the  $f_l$ , kindly furnished to us by Kees Rinzema,<sup>25</sup> we calculated both the intensity curves and  $\kappa_0$  by the transfer matrix method.<sup>21</sup> The results were in complete agreement with those of Rinzema *et al.*<sup>9</sup> Though they did not address the question discussed in this paper, one can calculate  $D$  and  $\alpha$  from their published results. We find  $\alpha = 0.55$  for their Case 1 and  $\alpha = 0.59$  for their Case 2. Thus their experiments show a clear absorption dependence for  $D$ .

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Address correspondence to Raphael Aronson, 64 Burnett Terrace, West Orange, New Jersey 07052. Phone, 973-325-3342; fax, 973-325-1089; e-mail, R1aron@aol.com.

## REFERENCES AND NOTES

1. R. L. Barbour, H. Graber, R. Aronson, and J. Lubowsky, "Model for 3-D optical imaging of tissue," in *Proceedings of the International Geoscience and Remote Sensing Symposium* (Institute of Electrical and Electronics Engineers, Piscataway, New Jersey, 1990), Vol. II, pp. 1295–1399.
2. A. G. Yodh and B. Chance, "Spectroscopy and imaging with diffusing light," *Phys. Today* **48**(3), 34–40 (1995).
3. S. R. Arridge and J. C. Hebden, "Optical imaging in medicine: II. Modelling and reconstruction," *Phys. Med. Biol.* **42**, 841–853 (1997).
4. M. Bassani, F. Martelli, G. Zaccanti, and D. Contini, "Independence of the diffusion coefficient from absorption: experimental and numerical evidence," *Opt. Lett.* **22**, 853–855 (1997).
5. K. Furutsu and Y. Yamada, "Diffusion approximation for a dissipative random medium and the applications," *Phys. Rev. E* **50**, 3634–3640 (1994).
6. K. Furutsu, "Pulse wave scattering by an absorber and integrated attenuation in the diffusion approximation," *J. Opt. Soc. Am. A* **14**, 267–274 (1997).
7. T. Durduran, D. A. Boas, B. Chance, and A. G. Yodh, "Validity of the diffusion equation for small heterogeneities," in *Advances in Optical Imaging and Photon Migration*, R. R. Alfano and G. Fujimoto, eds., Vol. 2 of OSA Trends in Optics and Photonics Series (Optical Society of America, Washington, D.C., 1996), pp. 60–63.
8. T. Durduran, A. G. Yodh, B. Chance, and D. A. Boas, "Does the photon-diffusion coefficient depend on absorption?" *J. Opt. Soc. Am. A* **14**, 3358–3365 (1997).
9. K. Rinzema, L. H. P. Murrer, and W. M. Star, "Direct experimental verification of light transport theory in an optical phantom," *J. Opt. Soc. Am. A* **15**, 2078–2088 (1998).
10. See, for instance, S. Chandrasekhar, "Stochastic Problems in physics and astronomy," *Rev. Mod. Phys.* **15**, 1–89 (1943); M. C. Wang and G. E. Uhlenbeck, "On the theory of Brownian motion II," *Rev. Mod. Phys.* **17**, 323–342. Both of these papers are reprinted in *Selected Papers on Noise and Stochastic Processes*, N. Wax, ed. (Dover, New York, 1964).
11. See, for instance, J. R. Lamarsh, *Nuclear Reactor Theory* (Addison-Wesley, Reading, Mass., 1966), pp. 125–128.
12. E. W. Larsen and J. B. Keller, "Asymptotic solution of neutron transport problems for small mean free paths," *J. Math. Phys.* **15**, 75–81 (1974); E. W. Larsen, "Diffusion theory as an asymptotic limit of transport theory for nearly critical systems with small mean paths," *Ann. Nucl. Energy* **7**, 249–255 (1980).
13. K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967).
14. J. R. Mika, "Neutron transport with anisotropic scattering," *Nucl. Sci. Eng.* **11**, 415–427 (1961).
15. K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967), Table 4.2, p. 91.
16. K. M. Case, F. de Hoffmann, and G. Placzek, *Introduction to the Theory of Neutron Diffusion*, Vol. I (Los Alamos Scientific Laboratory, Los Alamos, N. Mex., 1953).
17. G. Holte, "On a method of calculating the density of neutrons emitted from a point source in an infinite medium," *Ark. Mat. Astron. Fys.* **35A**(36), 1–9 (1948). Holte's notation is somewhat different from ours.
18. I. Kuščer and N. J. McCormick, "Some analytical results for radiative transfer in thick atmospheres," *Transp. Theory Stat. Phys.* **20**, 351–381 (1991). This paper gives Holte's result<sup>17</sup> in the form where we quote here.
19. S. Chandrasekhar, *Radiative Transfer* (Dover, New York, 1960).
20. K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967), Chap. 7.
21. 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).
22. H. C. van de Hulst, *Multiple Light Scattering* (Academic, New York, 1980), Vol. 2, Chap. 10.
23. G. Zaccanti, Dipartimento di Fisica dell'Università degli Studi di Firenze, Via Santa Marta 3, 50139 Firenze, Italy (personal communication), 1998.
24. D. J. Durian, "The diffusion coefficient depends on absorption," *Opt. Lett.* **23**, 1502–1504 (1998).
25. K. Rinzema, Department of Physics/Institute for Physics Education, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands (personal communication, 1998).