

# Optical diffusion of continuous-wave, pulsed, and density waves in scattering media and comparisons with radiative transfer

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We discuss several outstanding theoretical problems in optical diffusion in random media. Specifically, we discuss which of several diffusion theories most closely approximates exact solutions of the equation of transfer. We consider a plane wave impinging upon a plane-parallel slab of a random medium as a model problem to compare the diffusion theories with a numerical solution of the equation of transfer for continuous-wave, pulsed, and photon density waves. In addition, we discuss the validity of the diffusion approximation for a variety of parameter settings to ascertain the diffusion approximation's applicability to imaging biological media. © 1998 Optical Society of America

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## 1. Introduction

Transport theory's equation of transfer is a well-accepted model for wave scattering in a random medium.<sup>1</sup> However, exact solutions are available for only a small class of special cases (isotropic scattering in infinite and semi-infinite domains), and thus analytical solutions for a wide variety of geometries and range of parameters that correspond to more physically relevant situations still remain to be determined. Many researchers have derived diffusion approximations by use of asymptotic analysis.<sup>1-8</sup> These approximate equations have the advantage of easily obtainable, closed-form solutions. In addition, there are significant amounts of experimental data that agree well with the solution of the diffusion equation.<sup>9</sup> However, the applicability of the diffusion approximation to many other physically relevant settings remains questionable. Experimental evidence shows that biological media are highly anisotropic<sup>10</sup> (asymmetry parameter values greater than 0.9), and thus a careful investigation is necessary to determine the diffusion approximation's applicability

to highly anisotropic media. Furthermore, a question remains as to which of the several diffusion equations most closely approximates the solution given by the equation of transfer.

In this paper we address questions that pertain to the diffusion approximation of the equation of transfer for applications in biomedical imaging. We numerically solve the equation of transfer for the plane-parallel problem and compare the existing diffusion theories to determine which of several theories most closely approximates the equation of transfer. In doing this we determine the validity of the diffusion approximation for optically imaging biological media. Some numerical results have been obtained for the case when the refractive index of the background medium differs from that of the surrounding medium.<sup>11</sup> To evaluate the diffusion approximation's validity simply and effectively, we consider only the idealized case of index-matched boundary conditions. We perform these comparisons for continuous-wave, pulsed, and photon density waves.

## 2. Transport Theory

Transport theory models wave scattering by describing the transport of power through the medium. The fundamental quantity in transport theory is the specific intensity,  $I(\mathbf{r}, \hat{s})$ , which has units of  $\text{Wm}^{-2}\text{sr}^{-1}\text{Hz}^{-1}$ . In general the specific intensity is a function of the position vector in 3-space,  $\mathbf{r} = (x, y, z)$ , and the unit direction vector,  $\hat{s} = (\theta, \phi)$ , where  $\theta$  is the polar angle and  $\phi$  is the azimuthal angle. If we consider the plane-parallel problem (Fig. 1) with an inci-

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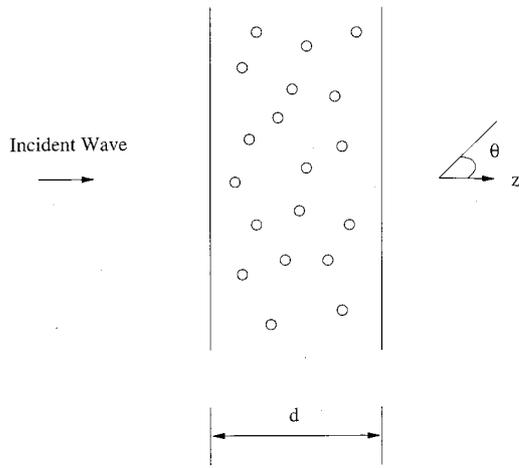


Fig. 1. Diagram of the plane-parallel problem.

dent wave directed normally to the slab, the governing equation for the specific intensity, the two-frequency equation of transfer or radiative transfer equation, can be reduced to having only three variables<sup>1</sup>: the frequency difference of the two frequencies,  $\omega_d = \omega_1 - \omega_2$ , the cosine of the polar angle,  $\mu = \cos \theta$ , and the optical depth,

$$\tau = \rho \sigma_t z, \quad (1)$$

where  $\rho$  is the number density of particles in the medium and  $\sigma_t$  is the total scattering cross section. Therefore the resultant nondimensional two-frequency equation of transfer for the diffuse component of the specific intensity from the narrow-band approximation takes the form

$$\mu \frac{dI(\tau, \mu)}{d\tau} + \left(1 - i \frac{\omega_n}{\tau_0}\right) I(\tau, \mu) = \frac{W_0}{2} \int_{-1}^1 p_0(\mu, \mu') \times I(\tau, \mu') d\mu' + \epsilon_{ri}(\tau, \mu), \quad (2)$$

where  $\tau_0$  is the maximum optical depth,  $W_0$  is the single-scattering albedo, and

$$\omega_n = \omega_d t_0, \quad t_0 = d/c \quad (3)$$

is the nondimensionalized frequency difference scaled by the characteristic time  $t_0$ , where  $d$  is the thickness of the slab and  $c$  is the group speed of the wave.

The kernel of the integral operator is defined as

$$p_0(\mu, \mu') = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2\pi} \int_0^{2\pi} p(\mu, \phi, \mu', \phi') d\phi d\phi', \quad (4)$$

where

$$p(\mu, \phi, \mu', \phi') = \frac{1 - g^2}{(1 + g^2 - 2g \cos \xi)^{3/2}} \quad (5)$$

is the Henyey–Greenstein phase function,

$$\cos \xi = \mu \mu' + \sqrt{1 - \mu^2} \sqrt{1 - \mu'^2} \cos(\phi - \phi') \quad (6)$$

is the cosine of the angle between the incident and the scattered wave vectors, and

$$g = \frac{\left[ \int_{4\pi} p(\mu, \phi, \mu', \phi') \cos \xi d\mu' d\phi' \right]}{\left[ \int_{4\pi} p(\mu, \phi, \mu', \phi') d\mu' d\phi' \right]} \quad (7)$$

is the mean cosine of the phase function or the asymmetry parameter.

The source term,  $\epsilon_{ri}$ , comes from the incident plane wave of unit flux directed normally to the slab:

$$\epsilon_{ri}(\tau, \mu) = \frac{1}{4\pi} p_0(\mu, 1) \exp(-\eta\tau), \quad (8)$$

where

$$\eta = 1 - i(\omega_n/\tau_0). \quad (9)$$

To solve Eq. (2) we need to prescribe boundary conditions. For the plane-parallel problem we assume that no incoherent light enters into the slab. Thus the only source of light is from the incident intensity. Therefore

$$\begin{aligned} I(\tau = 0, \mu) &= 0, & 0 < \mu \leq 1, \\ I(\tau = \tau_0, \mu) &= 0, & -1 \leq \mu < 0. \end{aligned} \quad (10)$$

With these boundary conditions we now have a well-posed mathematical problem.

### 3. Diffusion Approximation

As light propagates through a random medium, we assume that the specific intensity develops a nearly isotropic angular distribution because of the profound multiple scattering effects. This is the basic assumption of the diffusion approximation, and it allows us to consider the specific intensity as an asymptotic expansion of Legendre functions<sup>2</sup>:

$$I(\mathbf{r}, \hat{s}) = U_d(\mathbf{r}) + \frac{3}{4\pi} \mathbf{F}_d(\mathbf{r}) \cdot \hat{s} + \dots, \quad (11)$$

where

$$U_d(\mathbf{r}) = 1/2 \int_{4\pi} I(\mathbf{r}, \hat{s}) d\Omega \quad (12)$$

is the averaged intensity ( $d\Omega$  is the elementary solid angle in direction  $\hat{s}$ ) and

$$\mathbf{F}_d(\mathbf{r}) = \int_{4\pi} I(\mathbf{r}, \hat{s}) \hat{s} d\Omega \quad (13)$$

is the flux vector. Furthermore, we assume that

$$|\mathbf{F}_d(\tau)| \ll U_d, \quad (14)$$

which corresponds to the angular distribution's being nearly isotropic.

These assumptions yield a diffusion equation for

the plane-parallel problem that takes the nondimensional form

$$\frac{d^2 U_d(\tau)}{d\tau^2} + \kappa^2 U_d(\tau) = Q_0(\tau), \quad (15)$$

where

$$\kappa^2 = 3 \left\{ \alpha \frac{\omega_n^2}{\tau_0^2} + i \frac{\omega_n}{\tau_0} [W_0(1-g) + \beta(1-W_0)] - (1-W_0)[W_0(1-g) + \gamma(1-W_0)] \right\} \quad (16)$$

and  $\alpha$ ,  $\beta$ , and  $\gamma$  are parameters that correspond to the various diffusion theories.<sup>6</sup> These diffusion theories are summarized in Table 1.

The contribution from coherent sources is defined as

$$Q_0(\tau) = \frac{3}{4\pi} W_0 [gW_0 - \eta(1+g)] \exp(-\eta\tau). \quad (17)$$

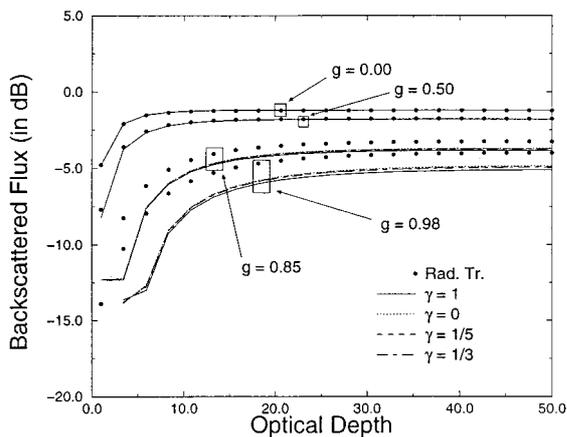
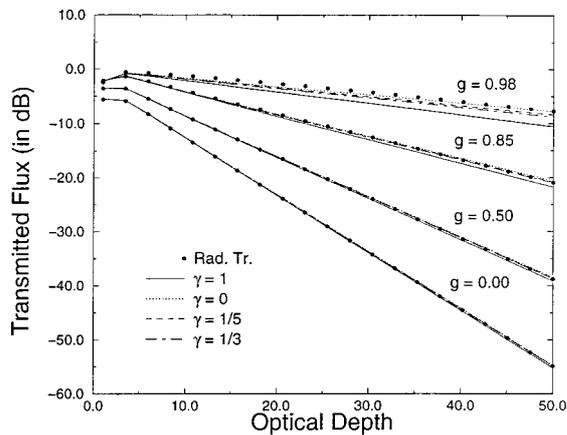


Fig. 2. Continuous wave: transmitted and backscattered fluxes for  $W_0 = 0.99$  and  $d = 3.0$  cm. Here and in subsequent figures, Rad. Tr. means radiative transfer.

Table 1. Parameter Values for the Various Diffusion Theories

Author of Theory	Abbreviation for Theory	Parameter		
		$\alpha$	$\beta$	$\gamma$
Ishimaru <sup>a</sup>	D1	1	2	1
Furutsu and Furutsu and Yamada <sup>b</sup>	D2	0	0	0
Polishchuk <i>et al.</i> <sup>c</sup>	D3	1/5	2/5	1/5
Durian and Rudnick <sup>d</sup>	D4	1/3	2/3	1/3
Patterson <i>et al.</i> <sup>e</sup>	D5	0	1	1

<sup>a</sup>Refs. 2 and 3.

<sup>b</sup>Refs. 4 and 5.

<sup>c</sup>Ref. 6.

<sup>d</sup>Ref. 7.

<sup>e</sup>Ref. 8.

On solving Eq. (15), we can determine the flux vector from the relation

$$\nabla U_d = \frac{3}{4\pi} (gW_0 - \eta) \mathbf{F}_d + \frac{3}{4\pi} gW_0 \exp(-\eta\tau) \hat{z}. \quad (18)$$

To solve Eq. (15) we need to prescribe boundary conditions that correspond to those defined in Eqs. (10). However, only approximate conditions exist,

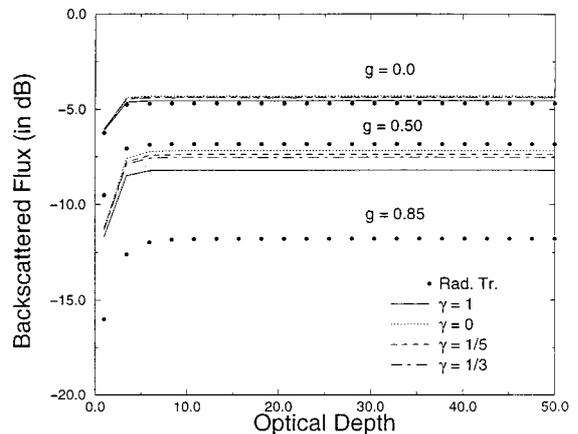
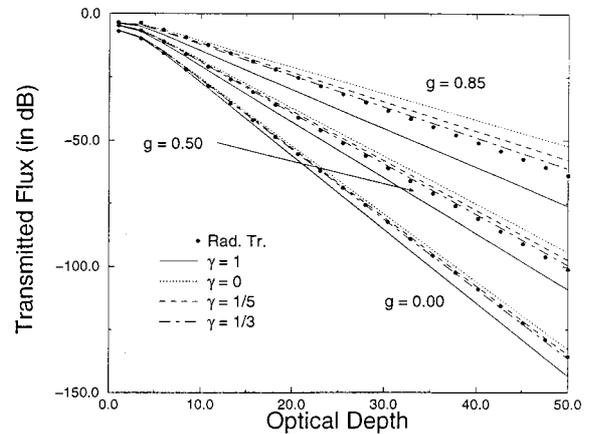


Fig. 3. Continuous wave: transmitted and backscattered fluxes for  $W_0 = 0.85$  and  $d = 3.0$  cm.

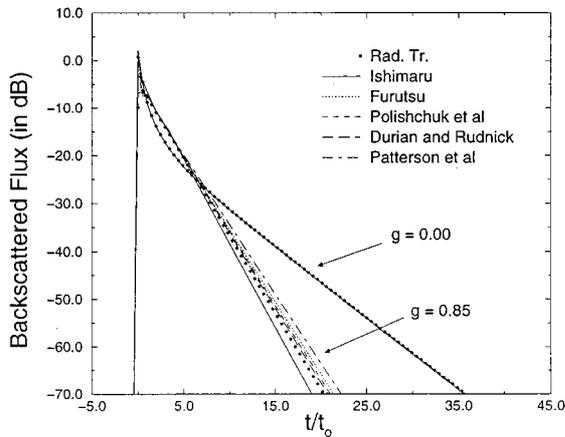
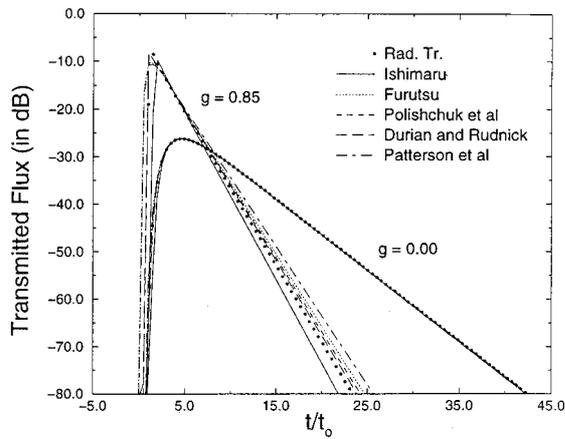


Fig. 4. 10-ps pulse: amplitude of transmitted and backscattered fluxes for  $W_0 = 0.99$ ,  $d = 3.0$  cm, and  $t_0 = 100$  ps.

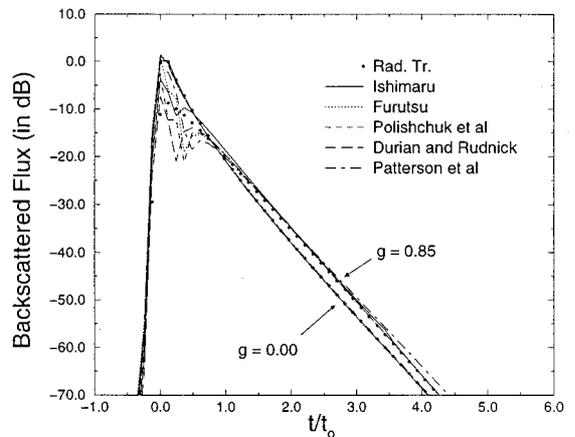
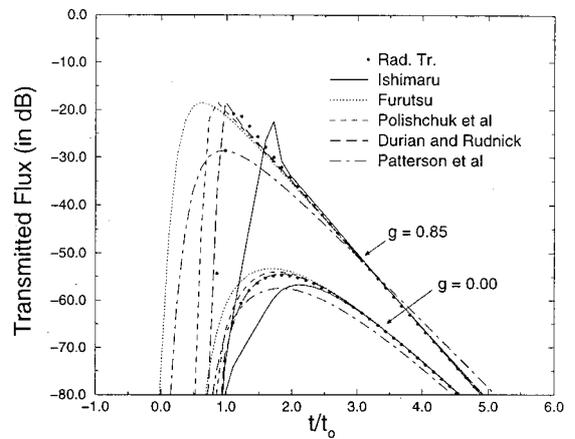


Fig. 5. 10-ps pulse: amplitude of transmitted and backscattered fluxes for  $W_0 = 0.85$ ,  $d = 3.0$  cm, and  $t_0 = 100$  ps.

which state that the total flux directed in toward the medium is zero and yields the Robin conditions<sup>2</sup>

$$\begin{aligned}
 U_d - h \frac{dU_d}{d\tau} + \frac{1}{2\pi} Q_1 &= 0, & \tau = 0, \\
 U_d + h \frac{dU_d}{d\tau} - \frac{1}{2\pi} Q_1 &= 0, & \tau = \tau_0,
 \end{aligned} \quad (19)$$

where

$$h = 2/3(gW_0 - \eta)^{-1}, \quad (20)$$

$$Q_1(\tau) = \frac{gW_0}{(gW_0 - \eta)} \exp(-\eta\tau). \quad (21)$$

Now, with Eqs. (15) and (19), we have a complete mathematical description of the diffusion equation for the plane-parallel problem. Closed-form solutions to the diffusion equation are easy to obtain, which makes the diffusion approximation an attractive alternative to solving Eq. (2). However, the diffusion approximation may not be appropriate for many situations that are physically relevant to imaging biological media. Therefore we compare the solutions of Eq. (15) with the

numerical solution of Eq. (2) to test the validity of the diffusion approximation.

#### 4. Numerical Results

To solve Eq. (2) we use the finite-element Galerkin method,<sup>12</sup> which handles highly anisotropic media with relatively low computational cost. The transmitted and backscattered fluxes,

$$F_T = 2\pi \int_0^1 I(\tau_0, \mu) \mu d\mu, \quad (22)$$

$$F_B = 2\pi \int_{-1}^0 I(0, \mu) \mu d\mu, \quad (23)$$

are calculated by quadrature.

Inasmuch as the diffusion approximation can be thought of as a limiting process toward an isotropic angular distribution, we suspect that the diffusion approximation works best for nearly isotropic media with an albedo near unity at large optical depths:

$$g \rightarrow 0, \quad W_0 \rightarrow 1, \quad \tau_0 \gg 1. \quad (24)$$

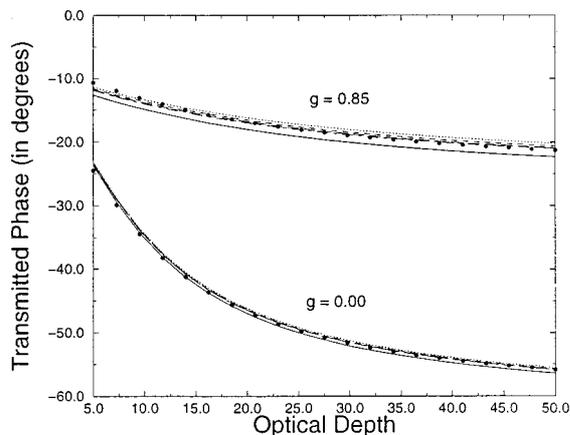
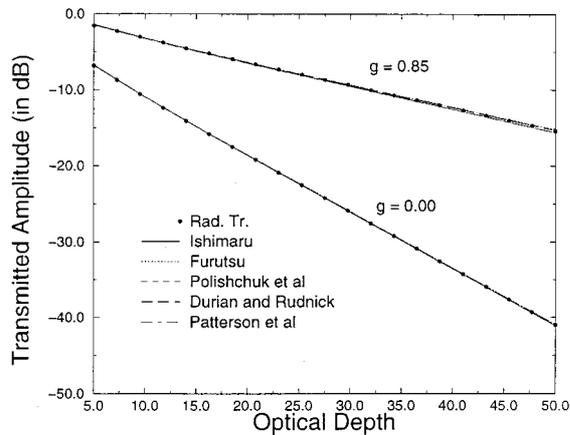


Fig. 6. Density wave: amplitude and phase of transmitted fluxes for  $W_0 = 0.99$  and  $d = 3.0$  cm.

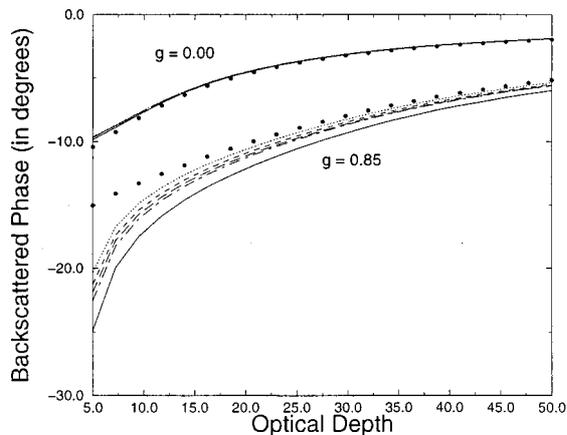
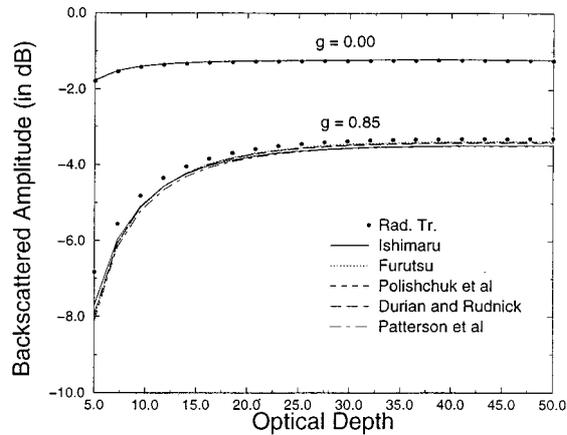


Fig. 7. Density wave: amplitude and phase of backscattered fluxes for  $W_0 = 0.99$  and  $d = 3.0$  cm.

The diffusion approximation should not be accurate for highly anisotropic ( $g \rightarrow 1$ ) and absorbing ( $W_0 \rightarrow 0$ ) media. Anisotropy and absorption impede the multiple scattering that is necessary for averaging out the angular distribution as the wave travels through the medium, especially at low optical depths. Furthermore, because the boundary conditions for the diffusion equation do not directly correspond to the boundary conditions for the radiative transfer equation, we expect deviations for lower optical depths where boundary effects are significant. Our numerical results are consistent with these ideas.

#### A. Continuous Waves

To calculate the solution for continuous waves we solve Eq. (2) for  $\omega_n = 0$  and  $d = 3.0$  cm. In Fig. 2 we consider  $W_0 = 0.99$ . For the transmitted flux, if the albedo is close to unity, then all the diffusion approximations are good for all asymmetry factors. Theory D4 (Table 1), which corresponds to  $\gamma = 1/3$ , appears to be closest to the radiative transfer solution for most values of  $g$  with a 0.1-dB deviation. Theory D2, which corresponds to  $\gamma = 0$ , agrees best for  $g = 0.98$ . All the other approximations are within a 0.5–1.0 dB deviation from the radiative transfer solution. For

the backscattered flux we observe that for  $g = 0$  and  $g = 0.5$  all diffusion approximations are good within 1 dB of the radiative transfer solution. However, for  $g = 0.85$ , all approximations deviate by 0.8 dB for large optical depths. For  $g = 0.98$ , all the approximations deviate by at least 2 dB for large optical depths.

In Fig. 3 we consider  $W_0 = 0.85$ . When we consider an absorbing medium, we observe that theory D4 is still the closest to the radiative transfer for the transmitted flux. The deviation from radiative transfer varies from less than 0.1 dB for isotropic media ( $g = 0$ ) to 0.3 dB for  $g = 0.9$  at  $\tau_0 = 50$ . Other diffusion approximations are within a few decibels, but the deviation increases to 12 dB for  $g = 0.9$  at  $\tau_0 = 50$ . For the backscattered flux, all approximations are within 0.5–1.0 dB for  $g = 0$  and  $g = 0.5$ . When  $g \geq 0.85$ , all the diffusion approximations are negative and thus give unphysical results and poor approximations to the radiative transfer solution.

#### B. Pulsed Waves

For our pulse calculations we consider a pulse width of 10 ps and slab thickness of 3 cm ( $t_0 = d/c = 100$  ps) at  $\tau_0 = 20$ . To obtain the solution in the time domain

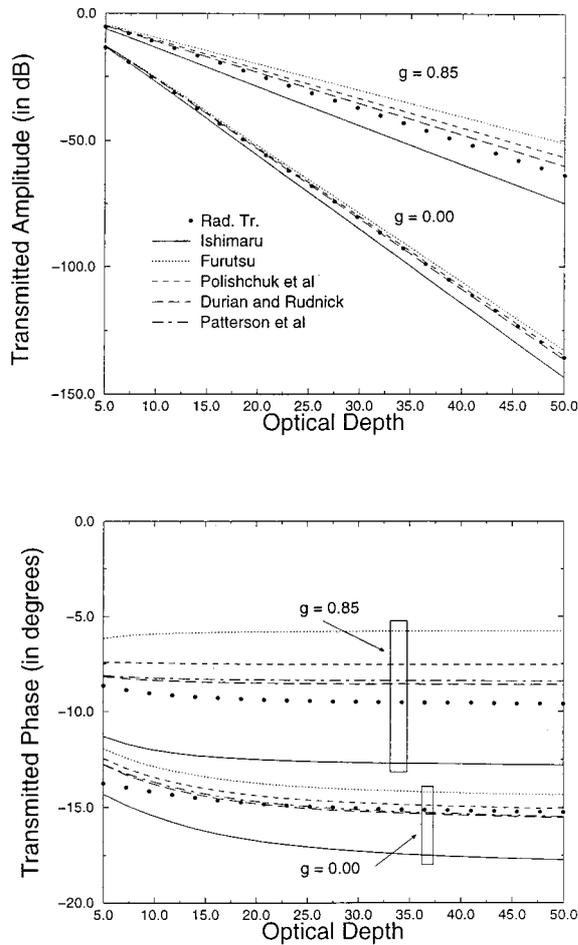


Fig. 8. Density wave: amplitude and phase of transmitted fluxes for  $W_0 = 0.85$  and  $d = 3.0$  cm.

we calculate the spectrum by solving Eq. (2) over a range of frequencies and convolving the spectrum with a Gaussian function of width  $T = 10$  ps, using fast Fourier transforms. The 10-ps Gaussian pulse measured at  $-70$  dB starts at approximately  $-0.4t_0$ . Both the width of the spectrum and the number of Fourier modes must be carefully considered when one is performing the fast Fourier transforms so the spectrum will be properly resolved.

In Fig. 4 we consider  $W_0 = 0.99$ . For the transmitted pulse in isotropic media ( $g = 0$ ), all the diffusion approximations are close to the radiative transfer. However, for short times, some differences can be observed. For short times, theories D2 and D5 start early to indicate true diffusion or the absence of a second derivative in time. For long times, all approximations are within 3 dB of radiative transfer. For  $g = 0.85$  there are considerable departures from radiative transfer in the short and long times. For the backscattered pulse in isotropic media, all the diffusion approximations are good. Again, some noticeable variations occur in short and long times for  $g = 0.85$ . Overall, theory D4 is closest to radiative transfer.

In Fig. 5 we consider an absorbing medium with  $W_0 = 0.85$ . For the transmitted pulse in isotropic media,

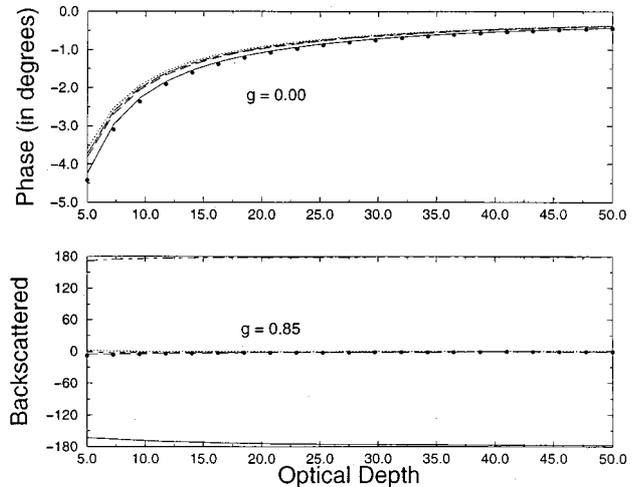
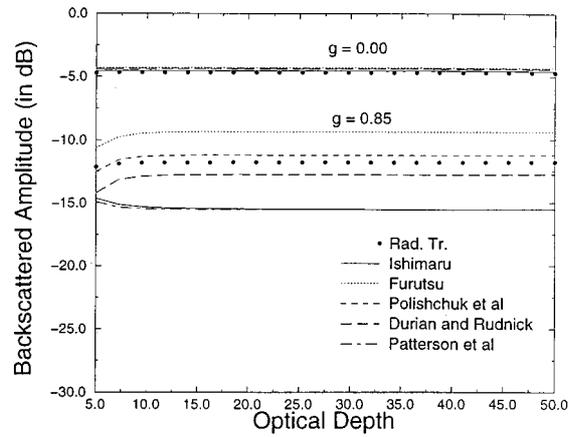


Fig. 9. Density wave: amplitude and phase of backscattered fluxes for  $W_0 = 0.85$  and  $d = 3.0$  cm.

theory D4 is closest. Other diffusion theories show some departures from radiative transfer for short times. For  $g = 0.85$ , the departures are evident for short times; again, theories D2 and D5 start early. For the backscattered pulse in isotropic media, all the diffusion approximations are good. For anisotropic media, considerable variations exist in the short time. Recall from the continuous-wave observations above that all the diffusion approximations are negative for this case. Analogously, the spectra of the diffusion approximations differ significantly, both qualitatively and quantitatively, from the spectrum given by the solution of the two-frequency equation of transfer. This difference can be seen through the presence of local minima just after the peak of the pulse. Because the spectra differ so greatly, we consider the presence of the local minima in the diffusion theories to be unphysical. Thus the diffusion approximation is inappropriate for this situation.

### C. Photon Density Waves

For our photon density wave calculations we consider a modulating frequency of 200 MHz ( $\omega_m = 0.125$ ) in a medium of thickness  $d = 3.0$  cm. In Figs. 6 (trans-

mitted) and 7 (backscattered), we consider  $W_0 = 0.99$ . For the transmitted and backscattered density waves in isotropic media, all the diffusion approximations are good. For  $g = 0.85$  we observe phase deviations of  $2^\circ$  for the transmitted density waves and significant deviations at small optical depths for the backscattered density waves. In Figs. 8 and Fig. 9 we consider  $W_0 = 0.85$ . For transmitted density waves (Fig. 8) in isotropic media, theory D4 is the best approximation because the other diffusion approximations have some departures in phase. For  $g = 0.85$ , the departure increases, but theory D4 remains the best. For backscattered density waves (Fig. 9) in isotropic media, the amplitudes of various approximations are within 0.5 dB, whereas the phases are within  $0.5^\circ$ . For  $g = 0.85$ , theories D3 and D4 are close to radiative transfer in amplitude; in phase, theories D1 and D5 are quite different from radiative transfer.

## 5. Conclusions

We have reviewed the theory of the diffusion approximation and compared the results from several existing diffusion equations with the numerical solution of the equation of transfer for continuous-wave, pulsed, and photon density waves under index-matched boundary conditions. The diffusion approximations work well for large optical depths, albedo values near unity, and asymmetry parameter values near zero. However, it is not necessarily appropriate to apply the diffusion approximation to highly anisotropic media (biological media) because the nearly isotropic angular distribution limiting process is greatly impeded by highly anisotropic scattering and absorption. Our examples above demonstrate these ideas.

For continuous-waves in a nearly lossless and isotropic medium, diffusion approximations are good for  $g \leq 0.85$ . We conclude that the diffusion approximation is no longer valid for asymmetry parameter values greater than  $g = 0.85$ . For pulses in a nearly lossless and isotropic medium, all diffusion approximations are good, but the departure of the diffusion approximations from the radiative transfer solution increases as  $g$  increases, especially for long times. In addition, for short times, the absence of the second derivative in theories D2 and D5 is noted. For density waves in a nearly lossless and isotropic medium, all the diffusion approximations are good. Again, departures are noticeable for anisotropic scattering.

Through the examples we have chosen, which correspond to parameters of interest for medical optics, theory D4 demonstrated the best performance overall. However, no conclusive statement can be made as to which of the several diffusion theories offers the best approximation to the equation of transfer, in general, because the individual performance of each of the diffusion theories changes with the parameter setting.

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