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Phase Velocity Limit of High-Frequency Photon Density Waves

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ABSTRACT

In frequency-domain photon migration (FDPM), two factors make high modulation frequencies desirable. First, with frequencies as high as a few GHz, the phase lag versus frequency plot has sufficient curvature to yield both the scattering and absorption coefficients of the tissue under examination. Second, because of increased attenuation, high frequency photon density waves probe smaller volumes, an asset in small volume *in vivo* or *in vitro* studies. This trend toward higher modulation frequencies has led us to reexamine the derivation of the standard diffusion equation (SDE) from the Boltzman transport equation. We find that a second-order time-derivative term, ordinarily neglected in the derivation, can be significant above 1 GHz for some biological tissue.

The revised diffusion equation, including the second-order time-derivative, is often termed the P1 equation. We compare the dispersion relation of the P1 equation with that of the SDE. The P1 phase velocity is slower than that predicted by the SDE; in fact, the SDE phase velocity is unbounded with increasing modulation frequency, while the P1 phase velocity approaches c/sqrt(3) in the high frequency limit. We emphasize that the phase velocity c/sqrt(3) is attained only at modulation frequencies with periods shorter than the mean time between scatterings of a photon, a frequency regime that probes the medium beyond the applicability of diffusion theory. Finally we caution that values for optical properties deduced from FDPM data at high frequencies using the SDE can be in error by 30% or more.

1. MOTIVATION

FDPM studies have been performed on living tissue at frequencies up to 3 GHz.¹ The phase lag versus frequency plot below a few hundred megahertz is close to a straight line. Since the plot necessarily goes through the origin, only one parameter, the slope of a straight line, is needed to describe the data. Independent values for both the scattering and absorption coefficients cannot be deduced. However, if data up to a few GHz is available, the plot has sufficient curvature to allow values for both coefficients to be extracted. Figure 1 contains a phase versus frequency curve for optical properties typical of biological tissue.

There is considerable interest in using photon density waves to probe smaller volumes both *in vivo* and *in vitro*. The greater attenuation of high frequency waves concentrates the probed volume in the vicinity of the source and detector fibers. Hence a number of factors are contributing to the trend toward higher modulation frequencies, and it is important to examine the validity at high frequencies of the

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Figure 1 - Phase lag versus modulation frequency for typical biological tissue.

approximations commonly made in deriving the standard diffusion equation (SDE) from the Boltzman transport equation.

2. THE P1 EQUATION

When the radiance can be expressed as an isotropic fluence rate ϕ plus a small directional flux \vec{j} , the transport equation reduces to the P1 equation:^{2,3}

$$D\nabla^2 \phi(\vec{r},t) - \mu_a \phi(\vec{r},t) - (1+3D\mu_a) \frac{1}{c} \frac{\partial \phi(\vec{r},t)}{\partial t} - \frac{3D}{c^2} \frac{\partial^2 \phi(\vec{r},t)}{\partial t^2} = -S(\vec{r},t) - \frac{3D}{c} \frac{\partial S(\vec{r},t)}{\partial t}$$
(1)

where the photon diffusion coefficient is given by $D = \frac{1}{3[(1-g)\mu_s + \mu_a]} = \frac{1}{3\mu_{tr}}$, and the linear

scattering and absorption coefficients, μ_z and μ_a , are the inverses of the mean free paths for scattering and absorption, respectively. The parameter g is the average cosine of the scattering angle, μ_{tr} is the transport scattering coefficient, and c is the speed of light in the medium. The source term $S(\vec{r}, t)$ represents power injected into a unit volume at \vec{r} .

The solution to the homogeneous P1 equation can be written as $\varphi(\vec{r},t) = \frac{\exp(-kr)}{r} \exp(i\omega t)$ where $k = k_{real} + i k_{imag}$ is given by:

$$k_{real} = \sqrt{(3/2)\mu_{a}\mu_{tr}} \sqrt{\sqrt{(1-\omega^{2}\tau\tau_{tr})^{2}+\omega^{2}\tau^{2}(1+\frac{\mu_{a}}{\mu_{\mu}})^{2}} + (1-\omega^{2}\tau\tau_{tr})}$$
(2)
$$k_{imag} = \sqrt{(3/2)\mu_{a}\mu_{tr}} \sqrt{\sqrt{(1-\omega^{2}\tau\tau_{tr})^{2}+\omega^{2}\tau^{2}(1+\frac{\mu_{a}}{\mu_{\mu}})^{2}} - (1-\omega^{2}\tau\tau_{tr})}$$

The mean time between scatterings is $\tau_{\mu} = 1/\mu_{\mu}c$ and the mean time till absorption is $\tau = 1/\mu_{a}c$. The angular frequency of modulation is ω .

At modulation frequencies sufficiently low that $\omega \tau_{tr} \ll 1$, the second-order time derivative in the P1 equation can be neglected with respect to the first-order derivative. The result is the standard diffusion equation (SDE):

$$D\nabla^2 \phi(\vec{r},t) - \mu_a \phi(\vec{r},t) - \frac{1}{c} \frac{\partial \phi(\vec{r},t)}{\partial t} = -S(\vec{r},t)$$
(3)

The solution to the homogeneous SDE has a complex wavenumber given by:

$$k_{real} = \sqrt{\frac{3}{2} \mu_a \mu_{tr}} \sqrt{\sqrt{1 + (\omega \tau)^2 + 1}} \qquad k_{imag} = \sqrt{\frac{3}{2} \mu_a \mu_{tr}} \sqrt{\sqrt{1 + (\omega \tau)^2 - 1}}$$
(4)

It is important to examine the approximation $\omega \tau_{tr} \ll 1$ for a range of optical properties. For typical biological tissue, $\mu_{tr} = 10$ /cm and the refractive index is approximately n = 1.40. At a modulation frequency of 1 GHz, $\omega \tau_{tr} = 0.029$ which validates the use of the SDE. However at higher frequencies or smaller values of μ_{tr} , the P1 equation may be required. For example, if $\mu_{tr} = 1$ /cm then at 1 GHz $\omega \tau_{tr} = 0.29$ and the second-order time derivative in the P1 equation cannot be neglected.

It is also important to examine the physical significance of $\omega \tau_{tr} = 2\pi \frac{\tau_{tr}}{T_{mod}}$ where T_{mod} is the

modulation period. Clearly the modulation period must be much longer than the mean time between scatterings τ_{tr} in order for diffusion theory to be applicable. The value $\omega \tau_{tr} = 0.29$ lies in the narrow regime where the P1 equation is required and the ratio of the modulation period to the scattering time $(T_{mod}/\tau_{tr} = 21.7)$ justifies a diffusion description.

To illustrate the differences in the solutions to the P1 and SDE equations, we plot the complex wavenumbers for $\mu_{tr} = 1$ /cm, $\mu_{a} = 0.013$ /cm, and n = 1.33 in Figure 2. The real and imaginary parts of the P1 wavenumber (solid lines) cross over at about 400 MHz, and the P1 imaginary part at 1 GHz is about 13% higher than the SDE imaginary part. The imaginary part of the wavenumber is proportional to the phase lag of photon density waves, and the real part accounts for attenuation. As we shall see later, this 13% difference in phase can result in more than 30% difference in the deduced values of optical properties.

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Figure 2 - Differences in complex wavenumber for solutions to the P1 and SDE equations.

It is interesting to note the differences in phase velocity of photon density waves predicted by the P1 and SDE equations. Plots of the dispersion relations for the two equations appear in Figure 3; the slopes of the lines drawn from the origin to the curves are the phase velocities. The SDE phase velocity approaches infinity with increasing frequency as has been noted by Svaasand et al.⁴ Ishimaru⁵ has pointed out that the P1 equation resembles a damped wave equation with a limiting phase velocity of c/sqrt(3). However, the magnitude of the second-order time derivative in the P1 equation is a factor of $\omega \tau_{tr}$ less than the magnitude of the first-order derivative. Only when $\omega \tau_{tr} > 1$ should the P1 equation assume the properties of a damped wave equation, so the phase velocity nears c/sqrt(3) only when the ratio of the modulation period to the scattering time (T_{mod} / τ_{tr}) is sufficiently small that diffusion theory is invalid.

It is clear from Figure 3 that the P1 phase velocity is always less than the SDE velocity at a given modulation frequency. At 1 GHz the P1 phase velocity is 8.6×10^9 cm/s which is only 66% of c/sqrt(3).

3. EFFECT ON THE DEDUCED OPTICAL PROPERTIES

The difference between the P1 and SDE curves for k_{imag} in Figure 2 amounts to 13% at a modulation frequency of 1 GHz. In order to determine what error would result in deduced values for optical properties, we simulated phase and modulation data using the P1 equation and fit that data with SDE expressions. The P1 simulated data with 5% noise is plotted in Figure 4.



Figure 3 - Dispersion relations for the P1 and SDE equations. The slope of the line drawn from the origin to the curve is the phase velocity.

The fit to the P1 phase data using an SDE fitting function (eqn. (4)) overestimated the transport scattering coefficient μ_{tr} by 24% and the absorption coefficient μ_{a} by 44%. On the other hand, the fit to the P1 modulation data using an SDE fitting function (eqn. (4)) underestimated μ_{tr} by 41% and μ_{a} by 44%. It is interesting to see that the reduced chi-squares for the fits are almost acceptable, increasing the likelihood that the fitting results would be given some credence. But the fitting results for the phase and modulation differ by more than a factor of two which certainly should raise a red flag.

We conclude that at modulation frequencies above 1 GHz and for values of μ_{tr} less than 10/cm, the P1 equation should be used to describe photon diffusion. The P1 expressions in eqn. (2) are only slightly more complicated than the SDE expressions in eqn. (4), so practically no additional effort is required.



Figure 4 - Simulated P1 phase and modulation data fit with SDE expressions.

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