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ANALYTIC PHASE FUNCTION FOR OCEAN WATER

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Analytic phase function for ocean water

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1. ABSTRACT

Using a modified form of the anomalous diffraction approximation we have been able to derive in closed form an analytic expression for the phase function of Mie scatterers integrated over an inverse power law (Junge) size distribution. The analysis explains the apparent singularity seen experimentally at the forward scattering angle. Simple relationships are also derived that relate the inverse power law as a function of scattering angle in the near forward direction to the power law of the size distribution. The parameters of the formula are the relative index of refraction and the inverse power of the size distribution. A comparison is given between the analytic formula and exact integration of the Mie scattering for spheres. This new phase function is used in the analysis of forward angle transmissometer-nephelometer data collected by DREV in the Arctic, Atlantic and Pacific.

2. INTRODUCTION

Many empirical formulae have been suggested as empirical fits to the phase function of oceanic waters[1−7]. They are often used in models of the light field and in analyses of optical system performance. Some work has also been carried out on fitting experimental phase functions to the exact Mie scattering solution numerically integrated over assumed or measured particle size distributions[8−12]. The former solutions have the advantage of simplicity and analyticity. They allow some progress to be made in the treatment of difficult multiple scattering problems. However the parameters used and the forms chosen are not directly based on the physics of the problem. In general, no information about physical parameters such as the mean index of refraction or the particle size distribution can be extracted. The latter exact Mie solutions allow one to extract some information about the physical parameters from the phase functions. These solutions, being purely numerical, are extremely inconvenient to use when dealing with light propagation problems. The present work tries to address this dichotomy by using a simple set of approximations to derive from the basic physics an analytic phase function whose parameters can be related to a limited set of physically meaningful quantities.

3. DERIVATION OF THE PHASE FUNCTION

In order to obtain the phase function of an ensemble of spherical particles one must perform the following integral.

$$\beta(\theta) = \int_0^\infty \pi r^2 \, Q_s(x) \, P(\theta, x) \, F(r) \, dr \qquad (1)$$

In equation 1, r is the particle radius and $x = 2\pi r/\lambda$, the particle size parameter. In this

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case λ is the wavelength of the illuminating source. $Q_s(x)$ is the scattering efficiency which is defined as the ratio of the particle scattering cross-section to the geometric cross-section. $P(\theta, x)$ is the single particle scattering function normalized to unity when integrated over 4π steradians. $F(r)$ is the particle size distribution function.

It has been noted that to a first approximation the measured particle size distributions in the ocean follow an inverse power law (Junge distribution).

$$F(r) = \frac{C}{r^\mu}$$

Assuming a distribution of this type it is instructive to write equation 1 in terms of the particle size parameter x.

$$\beta(\theta) = C\left(\frac{2\pi}{\lambda}\right)^{\mu-3} \pi \int_0^\infty Q_s(x)\, P(\theta, x)\, x^{2-\mu}\, dx \tag{2}$$

It is interesting that, as was noted by Morel[8], equation 2 predicts an inverse power relationship as a function of wavelength for the total scattering coefficient and that this is purely a property of the distribution function, independent of the particle shape. The only requirement is that the index also be independent of wavelength over the range of interest.

A second important conclusion can be drawn immediately from an analysis of equation 2: the phase function will be infinite in the forward direction ($\theta = 0$). This singularity occurs because in the large particle limit, $Q_s(x) = 2$ as required by Babinet's principle and $P(0, x) \propto x^2$. This last relationship is due to the fact that the width of the central forward diffraction peak of a finite object narrows inversely as the square of the size parameter and therefore the normalized amplitude of the scattering at $\theta = 0$ must increase as the square of x. It should be noted that this scaling is due to the wave nature of light and will apply even in the case of irregularly shaped finite particles with the proviso that the size parameter be replaced by some effective size parameter such as that of the volume equivalent sphere. Therefore, for any inverse power particle size distribution such that $3 \leq \mu \leq 5$, $\beta(0) \to \infty$.

From an analysis of equation 2 we can show that for small finite angles the scattering coefficient approaches infinity as an inverse power of θ. Chen[13] has recently shown that for large particles with modest indices of refraction

$$P(\theta, x) = N(x) p(2x \sin(\theta/2)) \tag{3}$$

to a good approximation. $N(x)$ is the normalization factor obtained when one integrates the scattering function over the sphere and $p(z)$ is the unormalized scattering function. If we now define two new variables $u = 2\sin(\theta/2)$ and $z = xu$ and substitute them in equation 2, we obtain:

$$\beta(\theta) = C\left(\frac{2\pi}{\lambda}\right)^{\mu-3} \pi \frac{1}{u^{3-\mu}} \int_0^\infty Q_s(z/u)\; N(z/u)\, p(z)\, z^{2-\mu}\, dz. \tag{4}$$

The angular dependence in the kernel of equation 4 is now contained in the normalization factor $N(z/u)$ and in $Q_s(z/u)$. As mentioned previously for large particles which dominate the scattering near the forward direction $Q_s = 2$ and $N(z/u) \propto z^2/u^2$. It therefore immediately follows by substitution of these expressions into equation 4 that in the near forward direction

$$\beta(\theta) \propto \frac{1}{u^{5-\mu}} \tag{5}$$

Since $u \to \theta$ for small values of θ the near forward scattering varies as an inverse power of θ This corresponds to the small angle scattering behavior seen experimentally[14]. This behavior at and near $\theta = 0$ means that when a perfect nephelometer is operated very near the forward direction it will measure its own diffraction limit as the point where a roll over from the inverse power law occurs.

The conclusions we have reached are different from those of Morel[8]. The discrepancy arises because he has not taken into account the x^2 normalization factor in $P(0, x)$. For $\mu = 5$ the rate of divergence of $\beta(0)$ as a function of the upper limit of the integral in equation 2 is logarithmic. It is therefore extremely difficult to verify convergence numerically by integrating the phase function given by a Mie code over a particle distribution. Increasing the upper limit of integration by an order of magnitude only increases $\beta(0)$ by a small factor. Given the limited computer resources available at the time, the statements by Morel about the numerical convergence of $\beta(0)$ are perfectly understandable.

The relative index of oceanic particles is generally close to unity. This is precisely the regime where anomalous diffraction theory applies[15]. A simple expression for $Q_s(x)$ can be obtained in this regime. For real values of the relative index n,

$$Q_s(x) = 2 - (4/\rho)\sin\rho + (4\rho^2)(1 - \cos\rho). \tag{6}$$

$\rho = 2(n-1)x$ is the phase difference between an unscattered ray and the central ray through the particle. Equation 6 predicts a series of gentle oscillations that ultimately damp down to a constant value of 2 for large ρ. Although $Q_s(x)$ has a relatively simple expression, it does not lead to a simple expression when one tries to further integrate equation 2. We therefore replace it by the following approximate expression.

$$Q_s(x) = \frac{\rho^2/2}{(1 + \rho^2/4)} \tag{7}$$

This expression has the same asymptotes as equation 6 for both small and large particle sizes but does not model the oscillations. The hope is that since we will be performing an integral over a Junge distribution the contribution of the oscillations will be minimized. More accurate approximations could be used but at the cost of increased complexity in the final result.

The phase function is more difficult to model even in the anomalous diffraction approximation. For spheres it leads in general to expressions that cannot be reduced to simple functions[15]. However, Van de Hulst has shown that in the limiting case of small ρ the functional form of the anomalous diffraction phase function reduces to the same functional form as that given by Rayleigh-Gans theory. In the opposite limit of large ρ, the anomalous diffraction phase function converges for moderate angles to the standard diffraction theory result. These results have recently been confirmed by Klett[16] and Chen[13]. Klett also shows that polarization is maintained in the anomalous diffraction approximation. This means that all phase functions for unpolarized light will have the standard multiplication factor of $(1+\cos^2\theta)/2$. Note that this factor is independent of particle size and can therefore be immediately taken outside the integral for $\beta(\theta)$. Both the Rayleigh-Gans and the diffraction formulae involve Bessel functions. As in the case of the extinction efficiency these do not lead to simple results when the integral is carried out in equation 2. We have chosen to approximate the Rayleigh-Gans expression by a function which models the central peak. The resulting normalized phase function is given by

$$P(\theta,x) = \frac{1}{4\pi}\frac{(1+4x^2/3)}{(1+u^2x^2/3)}. \tag{8}$$

$$u = 2\sin(\theta/2) \tag{9}$$

Substituting equations 7 to 9 into equation 2 , performing a partial fraction decomposition of the kernel and integrating leads to the following result

$$\beta(\theta) = C\pi\left(\frac{2\pi(n-1)}{\lambda}\right)^{\mu-3}\frac{1+\cos^2\theta}{8\sin(-\pi v)}\left[\frac{1}{(1-\delta^2)\delta^v}\right]$$
$$\left([v(1-\delta)-(1-\delta^v)]+\frac{4}{u^2}[(1-\delta^{v+1})-(v+1)(1-\delta)]\right). \tag{10}$$

Where

$$v = \frac{3-\mu}{2} \tag{11}$$

and

$$\delta = \frac{u^2}{3(n-1)^2}. \tag{12}$$

4. DISCUSSION

From equations 10 to 12 it is easy to show that in the limit of small angles we obtain the same result as equation 5. We notice that the constant of proportionality depends on all the parameters but the inverse power ν of the phase function near $\theta=0$ only depends on the inverse power μ of the particle size distribution function.

$$\nu = 5-\mu \tag{13}$$

The slope of the phase function near $\theta=0$ contains information only about the power law of the particle size distribution. As was mentioned previously the variation of the total scattering coefficient b will also be an inverse power γ of the wavelength.

$$\gamma = \mu-3 \tag{14}$$

Equations 13 and 14 can be used to relate the wavelength dependence of the total scattering coefficient to the logarithm of the slope of the phase function as a function of angle in the near forward direction.

$$\gamma = 2-\nu \tag{15}$$

We are currently attempting to verify this important relationship by using the experimental results of the NEARSCAT[4] transmissometer-nephelometer. Figure 1 is a graph of γ against ν where the solid line is the theory and the squares are the data points from NEARSCAT. The dashed line is the least squares fit to the data. The slope for the two lines are the same but the intercept has a positive offset of .25 which we cannot explain at this time.

Figure 2 is a graph of the results of equation 10 plotted against numerical computations using both the full anomalous diffraction model and calculations from a Mie code. The index was 1.05 and the particle size power law had an exponent of 3.5. The expressions were integrated using an order 512 gaussian integration scheme from $x = .2$ to $x = 4000.$. The results are not normalized. Both the Mie and the anomalous diffraction approximation were still not converged. In order to fully converge the computations special versions of the Mie code valid to $x = 100,000$ are required. We are currently working on improving the numerical algorithms in order to be able to compare our theory with properly converged Mie results. This illustrates the difficulty one can encounter when trying to estimate from theory the scattering behavior near $\theta = 0$.

Figure 3 is a graph of the experimental data of Petzold[14] for San Diego harbor. The solid line is a fit to the data using equation 10. We chose this data because the scattering is almost exclusively due to particles. In this case the contribution of the water background scattering is negligible. The value of μ in equation 10 was chosen by using the measured slope as a function of θ ($\nu = 1.346$) in equation 13. The index was varied to obtain a best visual fit ($n = 1.12$). The absolute values were normalized at $\theta = .1°$. The value of 1.12 for the mean index of refraction is compatible with the one given by Mie code integrations.

5. CONCLUSIONS

We have proven that for an inverse power particle size distribution there exists a singularity at $\theta = 0$ for all powers μ such that $3 \leq \mu \leq 5$. We have also shown that under mild restrictions, for small angles $\beta(\theta) \propto 1/\theta^{5-\mu}$. This leads to an interesting relationship between the inverse power of the small angle scattering and the inverse power of the total scattering coefficient as a function of wavelength. We have begun to verify this relationship using experimental data from our small angle nephelometer-transmissometer. We have derived a simple approximate parametric form for the oceanic phase function. We have attempted to compare this form with both Mie calculations and experimental data. Because of the difficult problems of numerical convergence our comparison with Mie results has met with limited success. We are currently trying to reformulate the numerical integration in a way that would allow direct comparisons to be made at more modest cost in computing time. The experimental fit gave encouraging results and equation 10 can be used for this purpose. The accuracy of the mean index values obtained is still up to debate at this time.

It should be noted in passing that the reality of the inverse power behaviour of scattering as a function of θ at small angles is a measure of the remarkable size extent of the Junge distribution. The reasons for the enormous apparent range of validity of this behavior are far from clear. Water turbulence, which would have an inverse power spectrum of $1/x^{11/3}$, could be involved. These effects need careful further study.

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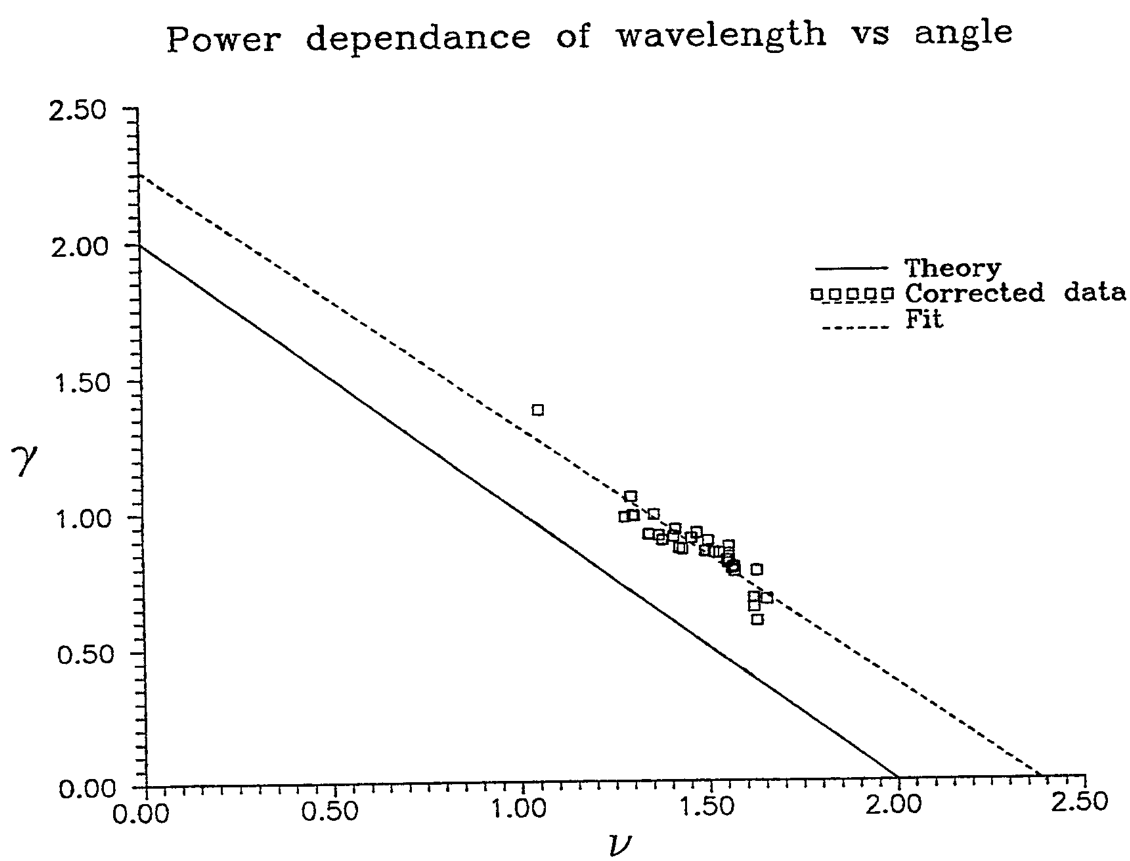

Figure 1. Plot of the inverse power γ of the total scattering coefficient as function of wavelength against the inverse power ν of small angle forward scatter.

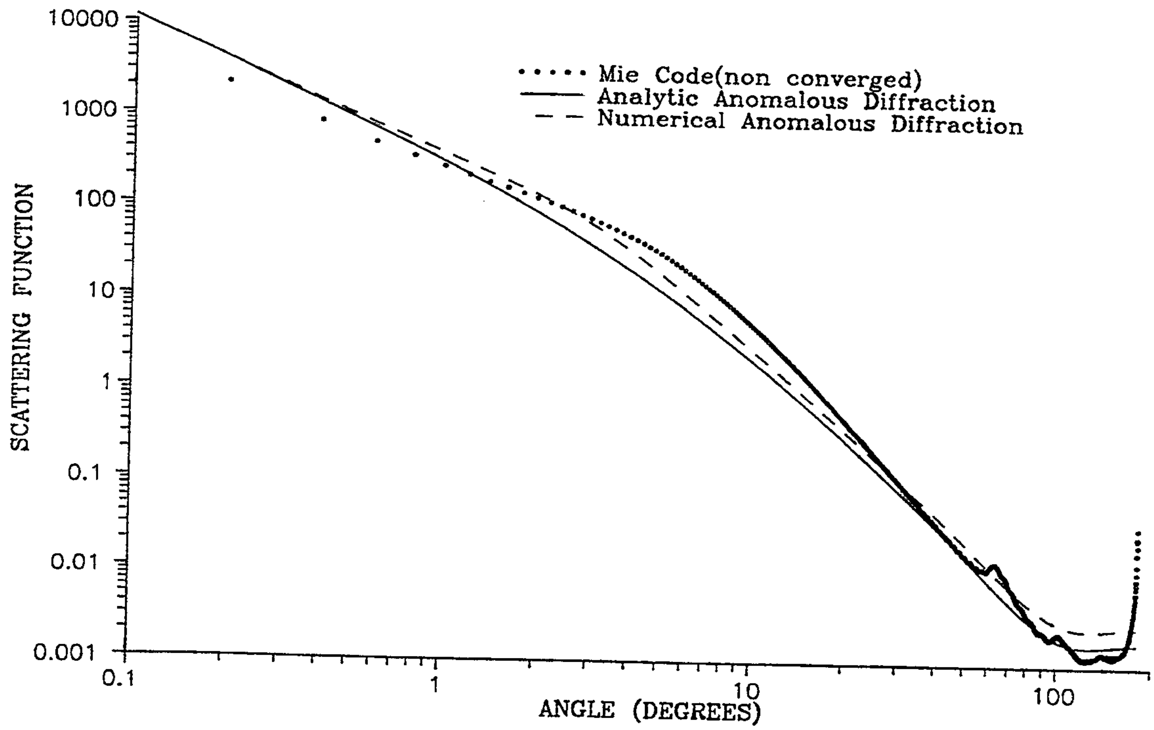

Figure 2. Comparison the analytic formula with the results of a numerically integrated Mie code and anomalous diffraction. ($\mu = 3.5, n = 1.05$)

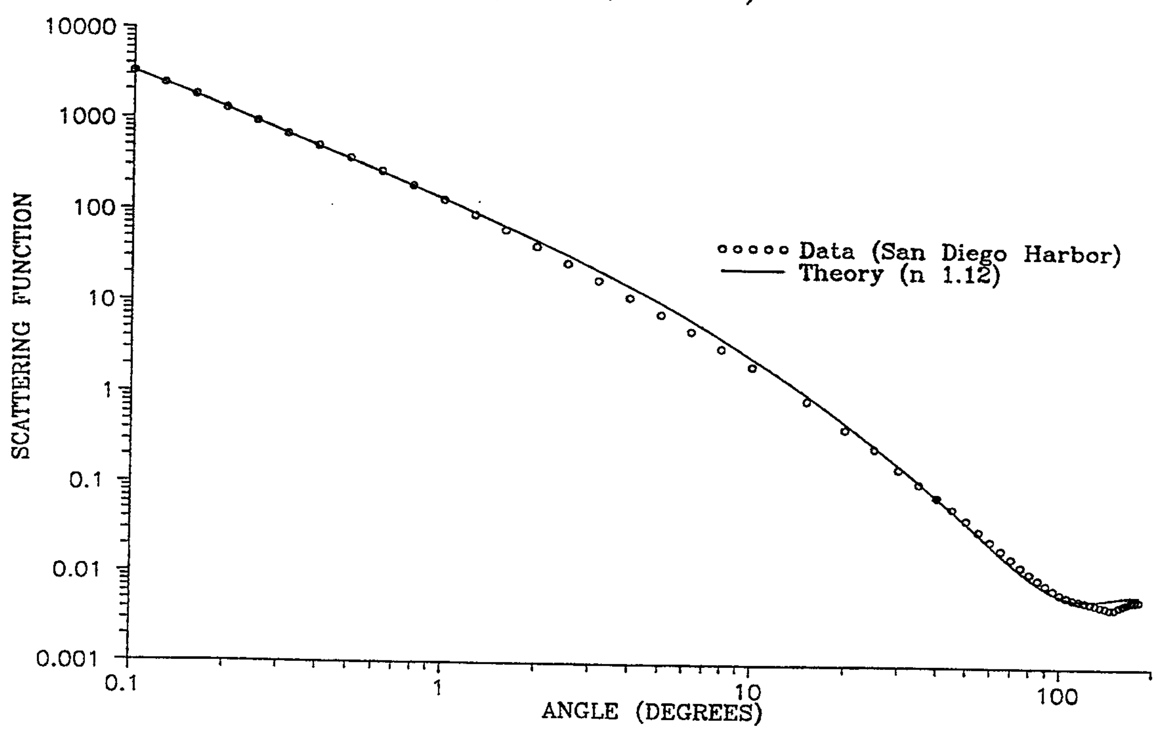

Figure 3. Comparison of the analytic formula with the Petzold data for San Diego harbor.