Beyond the Nutting Formula: Evaluation of Methods for Calculating Optical Density from Absorption and Scattering Cross Sections

Steven H. Kong[A] and Joel D. Shore[B]; Eastman Kodak Company; [A]Oakdale, MN and [B]Rochester, NY

Abstract

The Nutting formula is a simple relationship that estimates the optical density of a layer that contains a random distribution of absorbing particles. The only variables required are the extinction cross section of the particles and the number of particles per unit area. However, the Nutting formula is only accurate when light scattering is unimportant. More sophisticated methods for calculating the optical density that take into account light scattering are explored and compared.

Introduction

The optical density is an important measure for a variety of media. For example, the optical density for transmission is relevant for medical images, while the optical density for reflection is relevant for inkjet prints. A typical medium has both absorbers and scatterers. The optical properties of ordinary paper are dominated by light scattering. Conversely, the optical properties of a clear piece of dyed plastic are dominated by light absorption. In the case where there is negligible light scattering, the Nutting model can be used to calculate the optical density (OD) for the transmission of light through a dispersion of absorbing particles [1,2].

$$\mathrm{OD} = 0.434 n \sigma d \quad (1)$$

n is the number of particles per unit volume, d is the layer thickness, and σ is the extinction cross section of the particle. σ is often taken to be the projection area (or "geometric cross section") of the particle [2]. However, this is not accurate for small particles, so it is necessary to calculate the cross section [3]. For a particle that absorbs and scatters, $\sigma = \sigma_A + \sigma_S$, where σ_A is the absorption cross section and σ_S is the scattering cross section. If the particles have a significant scattering component, then Eq. 1 is only valid for specular transmission.

In cases where scattering dominates, paper for instance, the Kubelka-Munk (KM) approximation is typically used [4]. The attractiveness of the KM model is in its simplicity and utility. It is straightforward to calculate the absorption and scattering coefficients from the reflectance data. However, this method is less accurate when the absorption is too high, so there have been recent attempts to improve upon the KM theory [5]. This revised Kubelka-Munk (RKM) theory tries to account for the increased path length due to scattering.

Recently, the topic of light propagation in a turbid medium in the regime of significant absorption has become of great interest in both soft condensed matter physics and medical diagnostics [6]. Another area that could benefit from this recent work, and is of particular interest to the authors, is the calculation of the covering power for a dispersion of silver particles [7]. For example, small silver spheres can scatter and absorb light strongly [3].

There have been many approaches for modeling photon propagation in a turbid media. A phenomenological approach to the problem is to define a number of fluxes in the medium and set up differential equations to govern the radiation transfer between them [4]. The many-flux theory is the most generalized phenomenological theory. While it is theoretically useful, it is not practical. However, this approach becomes much more practical when the number of fluxes is limited. The simplest case is the one-flux theory, which results in Lambert's law and is essentially the same as the Nutting model. A specific case of the two-flux theory gives the very popular KM theory. Although not as popular, the four-flux theory can be very useful because it adds two directional fluxes. A specific case of the four-flux theory essentially gives a KM theory with a directional incident beam instead of a diffuse incident beam.

Assuming the particles are far enough apart to be treated independently and the light is incoherent, one can use a geometric optical approach to follow the path of the light between the scattering or absorption events. In this case, an accurate solution can be obtained using a random walk Monte Carlo Simulation [8]. While this method is useful as a benchmark, it is too time-consuming and unwieldy to be very practical. It is much more desirable to have a closed-form expression relating the total transmission and the cross sections of the particles. There have been many attempts to model the random walk nature of photon propagation in a turbid medium. A classic approach is to approximate the random walk as a diffusion problem [9,10]. However, this method is only accurate for relatively weak absorption, and the solutions violate causality [11]. Another method for modeling the random walk of photons in an absorbing medium that has gained prominence is the use of the telegrapher's equation, which has been shown to be a significant improvement over the diffusion equation [10-12]. More recently, there has been a proliferation of different methods recommended: The Orenstien-Uhlenbeck process [13], the cumulant approximation [14], and the Gaussian approximation [15]. Currently, there is no consensus on which is the best approach. For calculating the optical density of a turbid slab, we have decided to focus our attention on the telegrapher's equation because this method has been developed to a greater degree, is practical, and has given us good results.

In this paper, relationships for total transmission are derived for diffuse and normally incident light onto a slab containing a dispersion of particles, given the absorption and scattering cross sections for these particles. The derivations were carried out using solutions to the telegrapher's equation, and these solutions were evaluated by comparing them to solutions obtained by using the random walk Monte Carlo simulation, RKM theory, KM theory, the four-wave theory, the revised four-wave theory, and the Nutting model.

Results and Discussion

Diffuse Incident Light

The following time-independent form of the telegrapher's equation [6] was used for the case of a diffuse light source at $z = z_0$ and an infinite x-y slab occupying the region from $z = 0$ to $z = d$,

$$D'\frac{\partial^2 n}{\partial z^2} - ac\,n = -j_0\,\delta(z - z_0) \quad (1)$$

where

$$D' = \frac{c}{3(s + \beta a)} \quad (2)$$

and

n = number of photons per unit volume
a = absorption coefficient
s = scattering coefficient
c = speed of light
j_0 = current density of the light source.

In Eq. 2, β is a constant. When $\beta = 0$, Eq. 1 gives the diffusion approximation for photon propagation [6].

The general solution to Eq. 1 is

$$\begin{aligned} n(z) &= n_1(z) = A_1\sinh[q(z - z_0)] + B_1\cosh[q(z - z_0)] \quad z < z_0 \\ n(z) &= n_2(z) = A_2\sinh[q(z_0 - z)] + B_2\cosh[q(z_0 - z)] \quad z > z_0 \\ q &= \sqrt{3a(s + \beta a)} \end{aligned} \quad (3)$$

The boundary conditions applied are:

$$\begin{aligned} &n_1(z_0) = n_2(z_0) \\ &\left.\frac{\partial n_2}{\partial z}\right|_{z_0} - \left.\frac{\partial n_1}{\partial z}\right|_{z_0} = \frac{-j_0}{D'} \\ &j(0) = -\eta_1 c n_1(0) \\ &j(d) = \eta_2 c n_2(d). \end{aligned} \quad (4)$$

$j(z) \equiv -D'\,dn/dz$ is the current density. η_1 and η_2 are the average z-component magnitude of the unit velocity vectors for the transmitted photons at $z = 0$ and $z = d$, respectively. $\eta = 1/2$ for an isotropic distribution, and $\eta = 2/3$ for a Lambertian distribution. Note that the boundary conditions chosen here are different from those chosen by Durian and Rudnick [11].

The resulting diffuse transmittance at the front surface of the slab (T_1) and the back surface of the slab (T_2) are:

$$\begin{aligned} T_1(z_0) &= \frac{-j(0)}{j_0} \\ &= \frac{\eta_1 q\left(a\cosh[q(d - z_0)] + \eta_2 q\sinh[q(d - z_0)]\right)}{(\eta_1 + \eta_2)\,qa\cosh[qd] + (\eta_1\eta_2 q^2 + a^2)\sinh[qd]} \end{aligned} \quad (5)$$

$$\begin{aligned} T_2(z_0) &= \frac{j(d)}{j_0} \\ &= \frac{\eta_2 q\left(a\cosh[qz_0] + \eta_1 q\sinh[qz_0]\right)}{(\eta_1 + \eta_2)\,qa\cosh[qd] + (\eta_1\eta_2 q^2 + a^2)\sinh[qd]} \end{aligned} \quad (6)$$

For a diffuse light source at the front surface of the slab ($z = 0$), the diffuse transmittance equals $2*T_2(0)$. The factor of 2 is necessary because $T_2(0)$ is derived under the assumption that diffuse emission at z_0 occurs into both the forward and backward half-spaces; however, one conventionally assumes that a real diffuse light source placed at the front surface of the slab will emit only into the forward half-space.

Normally Incident Light

For normally incident light at $z = 0$, a continuum of diffuse light sources is effectively generated in the slab with a current density proportional to: $s\,\exp(-\varepsilon z_0)\,dz$. Here $\varepsilon = a + s$ is the extinction coefficient. The product of this term with $T_2(z_0)$ is integrated over z_0 and added to the specular component to obtain the total transmittance (T):

$$\begin{aligned} T = &\frac{\eta q s\exp[-\varepsilon d]\left((a\varepsilon + \eta q^2)(\exp[\varepsilon d] - \cosh[qd]) - q(\eta\varepsilon + a)\sinh[qd]\right)}{(\varepsilon^2 - q^2)\left(2\eta q a\cosh[qd] + (\eta^2 q^2 + a^2)\sinh[qd]\right)} \\ &+ \exp[-\varepsilon d] \end{aligned} \quad (7)$$

To obtain Eq. 7, η_1 and η_2 were set equal, therefore, the subscripts were dropped.

In the literature, β values of 0, 1/5, 1/3, and 1 have been recommended [6]. Eq. 7 gives the same numerical results as Eq. 5.7 in Ref. 11 if we choose $\eta = 1/2$ and $\beta = 1/3$. We have also found other values to consider for β. In the KM theory, the s=0 solution for the diffuse transmittance exponentially decays with the thickness of the slab, which is only approximately true. By forcing $T_2(0)$ to follow an exponential decay with the slab thickness in the limit s goes to zero, we obtain the following relationship for generating new potential values for β.

$$\beta = \frac{1}{3\eta^2} \quad (8)$$

This gives $\beta = 4/3$ for $\eta = 1/2$. In this paper, we use $\eta = 1/2$ and try several different values for β.

Comparisons

The optical density for diffuse light incident on a slab was calculated for two different values of εd (extinction coefficient times the slab thickness) and several different values of ad (absorption coefficient times the slab thickness) using the KM theory, RKM theory, diffusion model, telegrapher's model, and the random walk Monte Carlo simulation. In the Monte Carlo simulation, the Lambertian distribution was used to generate the diffuse incident beam.

For the RKM theory, the Kubelka-Munk parameters *S* and *K* were calculated from the optical coefficients *s* and *a* using the following relationships from Yang et al. [5]:

$$S = \mu \alpha s / 2 \tag{9}$$

$$K = \mu \alpha a \tag{10}$$

$$\alpha = \frac{1}{I_0} \int_0^{\pi/2} \int_0^{2\pi} I(\theta,\phi) \tan(\theta)\, d\theta\, d\phi \tag{11}$$

$$I_0 = \int_0^{\pi/2} \int_0^{2\pi} I(\theta,\phi)\, d\theta\, d\phi \tag{12}$$

$$\mu \approx \left(\frac{s^2}{a^2 + as} \right)^{1/4} \quad if \quad d\sqrt{K^2 + 2KS} >> 1 \tag{13}$$

In addition, μ=1 if $s^2 < a^2$+as. $I(\theta,\phi)$ is the radiant intensity (W/Sr) for light incident on a sublayer, where θ is the polar angle relative to the z axis, and ϕ is the azimuthal angle about the z axis. I_0 is the radiant power (W) incident on this sublayer. In general, α is a function of *z*, but in practice, α is treated as a constant. For a Lambertian distribution, α = 2. The KM theory is recovered when μ is set equal to one instead of as specified in Eq. 13.

After careful inspection of the solutions for transmittance obtained from the different methods, it was discovered that certain solutions we have obtained using the telegrapher's equation are algebraically equivalent to solutions obtained by KM theory and the four-flux theory, assuming we make the following modification to Eqs. 9 and 10:

$$S = \alpha_S s / 2 \tag{14}$$

$$K = \alpha_A a` \tag{15}$$

$$\alpha_S = \sqrt{\frac{3}{\beta}} \qquad \alpha_K = \sqrt{3\beta} \tag{16}$$

By allowing α to be different in the relationships for *S* and *K* and restricting their values with Eq. 16 and Eq. 8, the KM solution for the transmittance of diffuse light becomes equivalent to the solution ($2*T_2(0)$) we obtain using the telegrapher's equation. Under the same set of conditions, the four-flux solution for the transmittance of normally incident light also becomes equivalent to the solution (Eq. 7) we obtain using the telegrapher's equation.

The equivalence of the solutions we obtained for transmittance using the telegrapher's equation with solutions obtained by the KM and four-flux theories has some interesting implications. For instance, the relationship between the phenomenological parameters *K* and *S* with optical coefficients *a* and *s* have always been a weak point in KM theory, which Yang et al. attempted to address [5]. Typically, α is set equal to 2. The results above suggest that α should equal the square root of 3 if $\alpha_S = \alpha_K$. In addition, allowing α_S to differ from α_K can potentially expand the usefulness of the KM and four-flux theories. This also provides an easier means of utilizing some of the solutions of the telegrapher's equation because the four-flux theory and especially the KM theory are standard theories that have been fully developed.

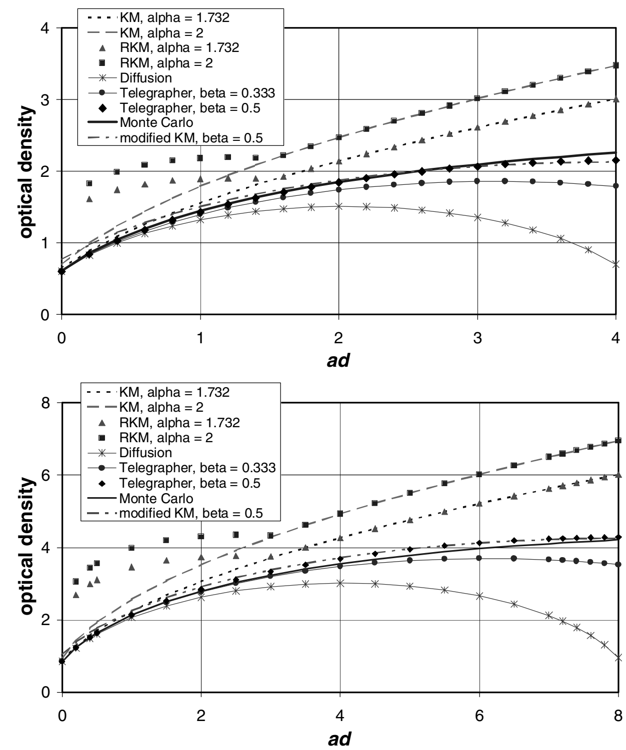

Figure 1. *Optical densities calculated for light diffusely incident on a slab with εd = 4 (top) and εd = 8 (bottom) using several different methods evaluated at several different values for ad. η = 1/2 for the telegrapher data.*

The results of the calculations show that the solution of the telegrapher's equation for $\eta = \beta = 1/2$, which does not satisfy Eq. 8., comes closest to the Monte Carlo data (Fig. 1). The agreement does degrade somewhat for lower εd values, but it is the best overall solution, especially for optical densities of interest. The results of the traditional KM model (i.e., α =2) give poor results, but are modestly improved when α is set equal to the square root of 3. A much greater improvement to the KM model is achieved when α_S is set equal to √6 and α_K is set equal to √(3/2). This solution of the modified KM model is equivalent to the solution of the telegrapher's equation for β = 1/2, η = √(2/3). The revised KM model gives the poorest results. Because the revised KM model was derived for paper applications, it might not be applicable to transmissive media.

The optical density for light normally incident on a slab was also calculated (Fig. 2). The calculations were made using the four-flux theory, revised four-flux theory, diffusion model, telegrapher's model, the Nutting model, and the random walk Monte Carlo simulation. The four-flux theory and the revised four-flux theory use the KM and RKM definitions for *S* and *K*, respectively. Further details on the KM and four-flux calculations can be found in Ref. 4.

The conclusions for normally incident light are similar to the conclusions for diffusely incident light. The telegrapher's equation for $\eta = \beta = 1/2$ gives the best overall results. The four-flux model for $\alpha = 2$ is marginally tolerable, but become reasonably good when α is set equal to the square root of 3. Results almost equivalent to the best case are achieved when α_S is set equal to $\sqrt{2}$ and α_K is set equal to $3/\sqrt{2}$ (not shown). This solution of the four-flux model using the modified KM parameters is equivalent to the solution of the telegrapher's equation for $\beta = 2/3$, $\eta = 1/\sqrt{2}$. Using the revised K and S in the four-flux theory gives poor results. The plots in Fig. 2 also show the regime where the Nutting model is valid. Using the extinction cross section in the Nutting model gives rough estimates for the optical density when the absorption coefficient is greater than the scattering coefficient.

The results for the reflectance calculations are not shown here. However, it is also found that certain solutions of the telegrapher's equation for reflectance can be expressed as solutions of the KM model and the four-flux model if those models are modified by using Eqs. 8, 14, 15, and 16. In the case of a Lambertian incident light, the telegrapher's equation for $\beta = 4/3$, $\eta = 1/2$ gives the best results and is equivalent to the KM model with $\alpha_S = 1.5$ and $\alpha_K = 2$. In the case of a collimated incident light, all of the models tested give good results.

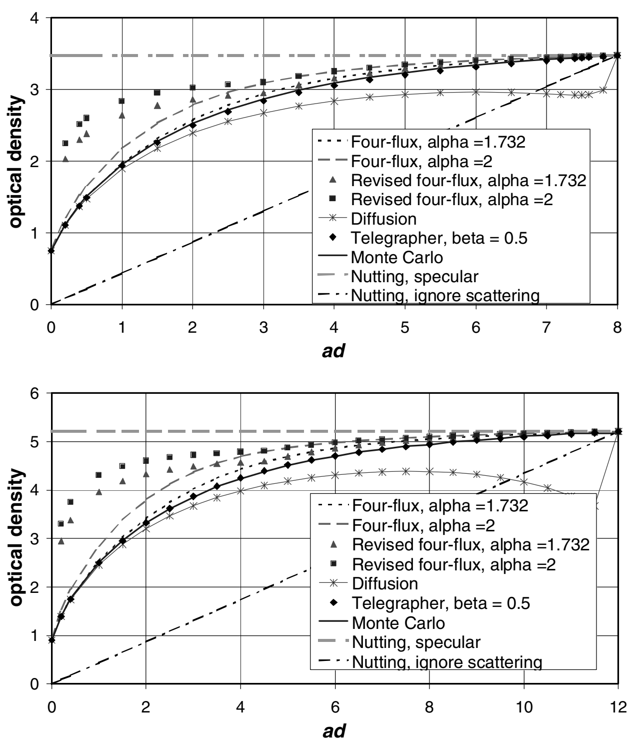

Figure 2. *Optical densities calculated for light normally incident on a slab with $\varepsilon d = 8$ (top) and $\varepsilon d = 12$ (bottom) using several different methods evaluated at several different values for ad. Telegrapher, $\beta = 1/3$ data are omitted to improve the visibility of the $\beta = 1/2$ data. The telegrapher, $\beta = 1/3$ case gives results that are a little worse than the $\beta = 1/2$ case. $\eta = 1/2$ for the telegrapher data.*

Summary

Several different methods were used to calculate the transmissive optical density of a slab given the absorption and scattering coefficients. A random walk Monte Carlo simulation was used to provide a benchmark solution. The calculation was made for light normally incident and diffusely incident on the slab. The results show that all of the models tested are superior to that of the Nutting model. However, the solution for the telegrapher's equation gives the best results. In addition, it was discovered that a class of solutions of the telegrapher's equation are also solutions of the Kubelka-Munk theory and four-wave theory, if we assume specific modified relationships between the phenomenological KM parameters (K and S) and the optical coefficients (a and s). The implication of this is that the utility of the KM theory and the four-wave theory can potentially be expanded. In addition, the application of the telegrapher's equation in certain cases can be simplified by using the KM theory and four-wave theory, because these methods have been fully developed.

References

[1] P.G. Nutting, Phil. Mag. 26, 423 (1913).

[2] J.C. Dainty and R. Shaw, Image Science (Academic Press, NY, 1974), p. 41

[3] D.R. Whitcomb, S. Chen, J.D. Shore, P.J. Cowdery-Corvan and K.A. Dunn, J. Imaging Sci. and Technol. 49, 370 (2005).

[4] H.G. Völz, in Industrial Color Testing (VCH, Weinheim, Germany, 1995), pg. 93.

[5] L. Yang and S.J. Miklavcic, Opt. Lett. 30, 792 (2005);
L. Yang and B. Kruse, J. Opt. Soc. Am. A 21, 1933 (2004);
L. Yang, B. Kruse and S.J. Miklavcic, J. Opt. Soc. Am. A 21, 1942 (2004); L. Yang, and S.J. Miklavcic, J. Opt. Soc. Am. A 22, 1866 (2005).

[6] D.J. Durian, Opt. Lett. 23, 1502 (1998).

[7] S.H. Kong and J.D. Shore, "Modeling the Impact of Silver Particle Size and Morphology on the Covering Power of Photothermographic Media", to be presented at ICIS, Rochester, NY (2006).

[8] J.J. DePalma and J. Gasper, Photogr. Sci. and Eng. 16, 181 (1972).

[9] A. Ishimaru, Wave Propagation and Scattering in Random Media (Academic, New York, 1978), Vol 1.

[10] A. Ishimaru, Appl. Opt. 28, 2210 (1989).

[11] D.J. Durian and J. Rudnick, J. Opt. Soc. Am. A 14, 235 (1997).

[12] R. Aronson and N. Corngold, J. Opt. Soc. Am. A 16, 1066 (1999).

[13] V. Gopal, S.A. Ramakrishna, A.K. Sood and N. Kumar, Prama J. of Phys., 56, 767 (2001).

[14] W. Cai, M. Xu, M. Lax and R.R. Alfano, Opt. Lett. 27, 731 (2002).

[15] K.R. Naqvi, preprint cond-mat/05044229 (2005) available at http://arxiv.org/.

Author Biography

Steven Kong is a Research Physicist with Eastman Kodak Company. He received his B.S. in applied physics and applied mathematics from the California Institute of Technology and a Ph.D. in physics from the University of Illinois at Urbana-Champaign. He began working in the field of photothermography at 3M in 1995. He is a member of IS&T and ANSI I3A, and serves in an ISO task group that addresses the image permanence of digital hard copies for medical imaging.