Predictive Modelling of Color Projection Quality I

Absorption and Scattering of Light by Pigment Particles in Toner Layers

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Introduction

It is well known that pigment dispersion is of importance to the color properties of toner films. Unfortunately, it has been difficult to quantitate pigment dispersion to the degree required for predictive models. Except for the general notion that smaller pigment is better, it has never been fully clear what the exact relationship between the size of these particles and the resulting color image properties is. This has resulted in the trial and error approach characteristic of the field.

This paper describes a comprehensive Mie scattering model to predict the transmission spectra of pigmented toner films as a function of detector collection angle, particle size and size distribution, layer thickness, and volume loading. The model requires two important input parameters: the pigment particle size and optical constants (complex refractive index: RI = n + ik). There were major problems inherent to each of these measurements which had to be solved in order to get our excellent predictive model for the key trends in color OHP transparencies. CIELAB coordinates a*, b*, c* and L*, projection efficiency, haze, pigment loading and TMA effects are predicted *a priori* within a few percent.

Particle Size Measurement

Good scattering predictions require good particle size measurements. The particle sizes were obtained by computerized image analysis of TEM images of sectioned toner samples, or by disc centrifuge measurement of pigments dispersed in water. Both methods gave good agreement in the absence of specific dispersion problems in water or toner. In particular, the volume median diameter (d_{50}) and geometric standard deviation (GSD), are the key size parameters of interest. Pigment particle size distributions are broad, with GSDs~2.0, and d_{50} = 50 –150 nm in "good" pigment dispersions; 300 –1000 nm in "poor" pigment dispersions.

Although image analysis of TEM micrographs from 100 nm thick toner sections has the advantage of sampling the actual pigment dispersion in toner, several problems had to be overcome. First, large particles had to be under weighted to adjust for particles larger than the section thickness. Second, the broadness of the distributions, combined with the need for the higher moment volume median, required counting 10^3-10^5 particles to achieve statistical significance. The necessary number of particles varies approximately as the 11th power of the GSD![1] Third, no single commercial image analysis software package was capable of all the image processing and analysis transformations required to generate the number, area and volume distributions of pigment particles suspended in toner films.

Pigment Optical Constants

The optical constants were obtained by Kramers-Kronig analysis of pigment pellet reflectance measurements by D. Tanner and J. Musfeldt at U. Florida.[2] The main problem to be overcome in this approach is that the Kramers-Kronig procedure used to convert measured pigment reflectance spectra into phase angle (θ), and hence refractive index ($RI = n(\theta) + i\,k(\theta)$) requires an integral over the entire frequency range, from 0 to infinity. Unfortunately, data below 200 nm (and, less significantly, above 20,000 nm) cannot be measured, and are usually obtained by extrapolation. Our approach was to vary an extrapolation parameter to minimize the least squares difference between the observed and predicted total toner transmission spectra. This optimizes the shape, but not the absolute intensity of the spectrum.

Mie Scattering Theory for OHP Layers

The sizes of pigment particles in color toners are such that when the toner is illuminated by light, the amount and angular distribution of the light scattered depends in a detailed way on the shape, size, orientation, and number density of the pigment. In this work the particles were assumed to be spherical, of uniform composition, and sufficiently separated that they can be considered as individual scatterers. These are reasonable assumptions, often found to apply for multi-particulate polydisperse assemblies of microcrystalline or irregular particles, where statistical averaging can smear the macroscopic properties to sphere equivalence.[3]

Figure 1 is a schematic of the general problem in overhead transparency projection. The pigmented toner layer is

illuminated from below. Light which passes through the transparency and falls within the lens capture angle, 2ϕ, is focussed onto the screen, yielding the image. Light scattered out of the collection angle is lost. Thus, the observed extinction is the sum of the absorption and light lost by scattering.

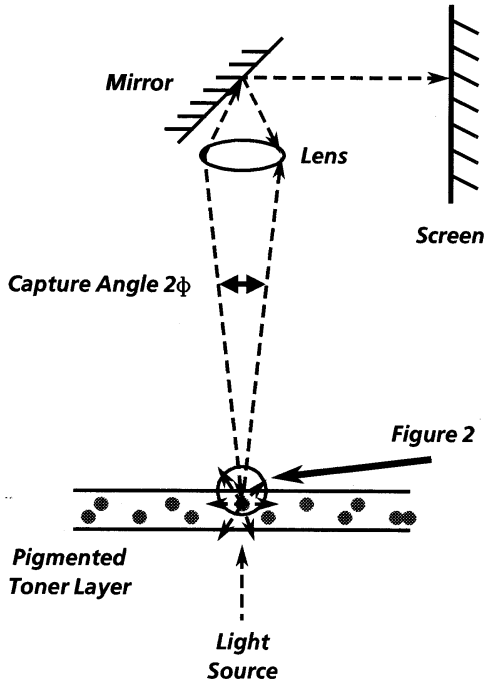

Figure 1. Schematic of Overhead Projector Optics.

Typical capture half angles for overhead projectors are in the 3.5-9° range, but the colour properties of overhead transparencies are measured with a color spectrometer, for example the Milton Roy Diano Match Scan II.[5] That instrument has a slightly different capture half angle, measured to be about ϕ=3.4° for the specular (P) spectrum, and ~90° for the diffuse (P+N) spectrum.

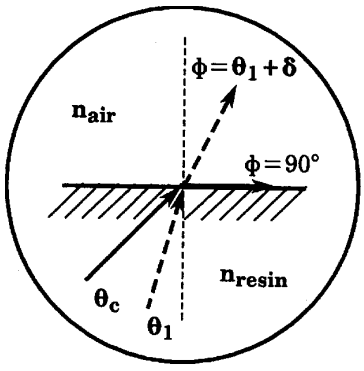

Figure 2. Details of Top Surface Refraction.

Figure 2 relates the capture half angle, ϕ, to the scattering angle in the resin, θ, by the refraction at the resin surface. Angles ϕ and 90° above the toner layer must be transformed into θ_1 and θ_c, respectively, for the integration of angular dependence. θ_c is the critical angle, above which total internal reflection occurs (~39° for resin with refractive index 1.6). Furthermore, to simplify the computation, we ignored the angular dependence of reflection at the resin–air boundary, and assumed that all light scattered at angles greater than the critical angle was eventually lost.

To model the physical characteristics of the system, requires a Mie scattering calculation[3,4] describing the fate of the unpolarized incident light in four terms: one for absorption and three for scattering, into the solid angles 0-θ_1, θ_1-θ_c, and θ_c-180°. The single particle Mie Theory allows us to compute all of these from the angular dependence of the scattered light. To generalize from the single particle calculation to a toner layer of polydisperse particles requires us to ignore multiple scattering effects, reflection and refraction. When this is done, we obtain predicted extinction coefficients, α_{ext}, such that:

$$T = \exp\left[-a_{ext}\phi_v L\right] \tag{1}$$

where: T is the transmittance; ϕ_v is the volume fraction of pigment in the toner layer; and L is the path length, or thickness of the toner layer (i.e. TMA). The extinction coefficients depend on the particle size and size distribution, the toner resin refractive index, the pigment optical constants, and the detector capture half angle, but do not depend on the pigment loading or sample thickness, so that:

$$a_{ext}(P+N) = a_{abs} + a_{sca}(\theta_c - 180°) \tag{2}$$

$$a_{ext}(P) = a_{ext}(P+N) + a_{sca}(\theta_1 - \theta_c) = a_{abs} + a_{sca}\,(\theta_1 - 180°) \tag{3}$$

The problem reduces to computing the additive absorption and scattering coefficients characteristic of a given pigment dispersion, then transmission spectra for any pigment loading and/or path length follow from Eq 1. For irregular top surfaces, a correction can be applied if the facet angle distribution is known.

Comparison with Experiment

This paper outlined the theory and measurement of key input parameters: particle size (state of pigment dispersion) and complex optical constants. The next paper, by E. Dalal, shows how successful the model is in practice. A third paper by H. Mizes describes surface facet angle distributions measured using atomic force microscopy.

References

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