Spectral Color Prediction by Advanced Physical Modelling of Toner, Ink and Paper, with Application to Halftoned Prints

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Abstract

A new spectral color prediction model for prints is presented, which is based on the combination of ray-tracing, Mie scattering and Monte Carlo simulation.

The wavelength dependent radiation transfer properties of ink or toner are determined by means of physically modelling the ingredients. The resin is described using optical constants, whereas the dyes use an absorption coefficient, and fluoresent re-emission probabilities. The scattering and absorption properties of pigments are described by the Mie theory, using realistic optical constants and particle size distributions.

Knowing the radiation transfer properties of the used materials, geometric objects like dots or layers are illuminated by a light source with adjustable spectral and directional characteristics. The angle and wavelength dependent reflectance and transmittance are obtained. The simulated reflection spectra agree well with measured data. Finally we combine printed patterns with a paper model containing scattering and fluorescent properties. In this way reflection spectra of printed samples are modelled succesfully.

The chosen approach is unique and more powerful than standard methods like Kubelka-Munk. Former difficult aspects of color prediction like surface gloss, angle-dependent scattering and fluorescence of dyes are an intrinsic outcome of this new model. The model is appropriate to make an accurate color prediction of halftoned prints.

Introduction

The color of a print depends on various factors. These factors are the ingredients and the fabrication process of the toner or ink, the printing process, the measurement geometry and the optical interaction between the toner or ink with each other and with the paper.

All these factors have complex interdependencies with respect to color, which researchers in imaging science are trying to understand. Examples of complex color issues are the relation between the optical behaviour of ingredients and the resulting color of a toner, and the physical or spatial interactions of printed toners with themselves and the paper.

To address these issues, several approaches can be taken. From a material point of view, the Kubelka-Munk[1] method can be used to determine the reflection of a scattering sample, where isotropic non-fluorescent scattering in up and down direction is used. From a halftone color prediction point of view, a number of methods can be used[2], of which Yule-Nielsen[3] and Clapper-Yule[4] are good examples. Recently, these two approaches are combined in more general models [Emmel et al.][5], using Kubelka-Munk with lateral scattering and fluorescence to describe ink on paper.

Although effort is made to further develop these models to fit particular cases, these methods are not generally applicable to the complex color issues discussed previously. These studies are all phenomenological, thus having a high dependency on the measurement arrangement. The description of the materials needs to be fitted on calibration samples. This results in free scalable parameters, which have no physical significance.

In order to have a model applicable to all factors influencing the color of a print, a new model is proposed and applied on toner systems. This model will be independent of the used measurement arrangement, and does not use free scalable parameters.

Methods

Outline of the Model:

The color impression of a print is the result of a rather complex propagation of radiation from the light source to the eye of the observer. Light rays incident on a print are reflected and transmitted at air-resin and resin-paper interfaces, scattered or absorbed by pigments and absorbed (and re-emitted if fluorescence is involved) by dyes. Radiation reaching the paper substrate is absorbed or reflected, with a spatial displacement depending on the light scattering properties of the paper ingredients.

In our color prediction approach we use a physical ray-tracing method containing the relevant objects mentioned above. The path of a ray emitted by the light source is followed in 3 dimensions. If the ray hits a surface or encounters a scattering event, we select a new direction based on physical probabilities and random number drawing (Monte Carlo). The simulation for one ray ends if it gets

absorbed or escapes to infinity. Figure 1 shows, as an example, the side view of such a Monte Carlo simulation of light propagation through paper.

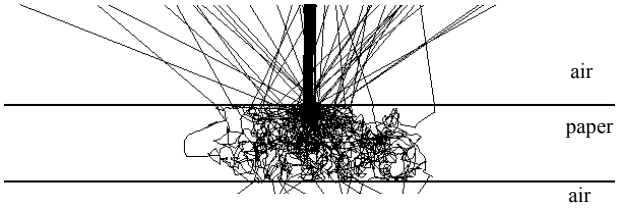

Figure 1. Paper simulation: A collimated beam is incident from the top in the center of the picture. The two horizontal lines indicate air-paper interfaces. At the interfaces the refractive index changes. In addition, the paper contains light scattering and fluorescent objects. Most rays travel in a kind of random walk through the paper, until they are absorbed or re-emitted at the top or bottom interface.

Using this technique we can easily handle arbitrary surface shapes (related to gloss and internal reflection), implement realistic scattering properties of pigments and paper, and investigate spatial effects of printed patterns.

For each wavelength we process several thousand rays to make sure that enough rays reach the detectors to have a satisfactory singal to noise ratio. This can be done on modern PC's with acceptable computational times.

The method is implemented using object oriented programming techniques. This makes it very easy to replace parts of the model by improved versions without the need to modify or re-consider the other objects.

Using the concept of light rays is a simplification. The alternative – a correct description by superposition of electromagnetic waves – leads to a strong coupling of all parts of the model. No applicable mathematical solutions exist for such kind of complex problems. On the other hand, we are quite confident that our ray-tracing approach is a good approximation for the treatment of spectral color prediction.

Simulation Details

A quantitative, physical model must be based on realistic optical constants of the materials in the system. The ray-tracing software used in this work can handle fixed data sets with imported literature data or flexible optical constant models. For resin, pigments and paper components we used models based on a superposition of a constant term and oscillators[6]. This turned out to be sufficient although more complex models are available. Dyes are described by absorption coefficients and fluorescent re-emission probabilities that have been obtained analyzing suitable experiments.

The reflection and transmission probabilities of macroscopic surfaces (air-resin, resin-paper, paper-air) are computed applying Fresnel's equations, taking into account the direction of the incoming ray. Surfaces can be flat or curved. The surface shape can be set by a user-defined function.

In between macroscopic interfaces rays move along straight lines, unless the volume contains scattering or absorbing particles. The ray-tracing software contains a module to compute the scattering and absorption properties of spheres (with multiple coatings or uncoated) according to Mie theory.[7] This was used for the pigments with realistic sphere radius distributions. The optical constants of each pigment type are determined analysing experimental spectra of simple model systems (pigments dispersed in resin layers on glass and aluminum).

In order to handle fluorescence the ray-tracing computations are started at the low wavelength end (300 nm) of the investigated spectral range (300 … 800 nm). In case of absorption by a fluorescent dye molecule the position of the ray and the wavelength of re-emission (higher than the wavelength of the absorption event) are stored temporarily. After all rays emitted by the light source have been processed for a certain wavelength, the program looks up if there are re-emission events to be considered for this wavelength. If so, rays are started at the stored positions with random direction. If all re-emitted rays are processed the next wavelength is considered. This way multiple absorption and re-emission steps are possible.

Experimental

Transmittance and reflectance measurements have been performed with a Perkin-Elmer Lambda 900 UV-Vis spectrophotometer. In addition, a Minolta Color-eye 7000A Spectrophotometer (d/8°, D65, 2° observer) has been used for reflectance measurements.

For fluorescence a SPEX fluorolog (Model FL3-22) has been used, for the quantum yield a Minolta CM-3800d bispectral spectrophotometer is used.

Due to the flexibility of the 3D ray-tracing approach we can setup model sceneries very similar to the experimental equipment we used. The spectral and directional characteristics of the light source are adjustable. The simulated detector signals are normalized exactly as the measured ones, and we can directly compare the spectra. During the descriptive phase only material parameters like optical constants or fluorescent emission features are varied in order to achieve agreement of models and measurements – no scalable free parameters without physical meaning are used.

For testing the applicability of the model in real toner-on-paper situations, an Océ CPS700 printer/copier is used. This printer produces images using 7 color toners (CMYKRGB).[8] All prints are made on Océ Colour Copy paper.

Results

Material Samples

Special fabricated samples are used to determine the optical behaviour of the used pigments and dyes. These samples consist of the material under investigation embedded in resin on a glass substrate. They are used to

measure the transmittance, while for reflectance an aluminum mirror is used to back the glass.

When a satisfying optical description of an ingredient is achieved, sample series with the new component are made with increasing concentration and thickness for validating purposes. The reflectance of these samples are measured and compared with the simulated reflectance of corresponding model systems, resulting in a typical $\Delta E < 3$.

An example of such a result is given in Figure 2. In this figure the increase in fluorescence with increasing absorption can be seen. Figure 2 proves that our simulation method is capable of correctly modelling fluorescence, making it applicable to fluorescent dyes and optical brighteners of paper.

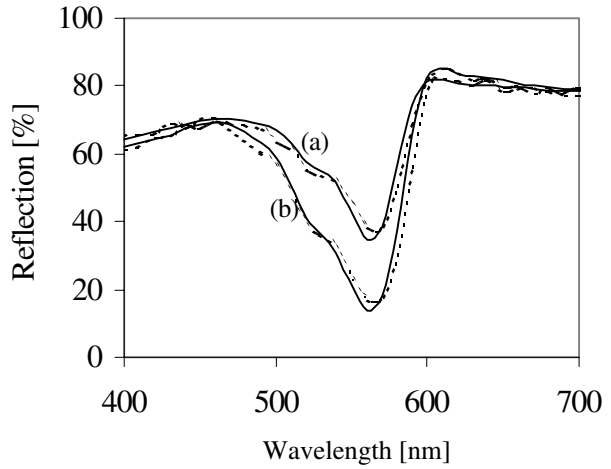

Figure 2. Measured (solid line) and simulated (dashed) reflection spectra of two layers of a magenta fluorescent dye with low (a) and high (b) concentration on glas backed with an aluminum mirror. The $\Delta E < 3$, and the dye absorbs light between 500 and 600 nm, and re-emits above 600 nm.

The next typical feature of our model is light scattering. The single scattering properties of the pigments are computed using Mie theory. Figure 3 shows the angle dependence of the scattering probabilities for a red pigment. Note that the characteristics are far from being isotropic, justifying the application of an advanced scattering theory.

The optical constants of the pigments have been determined, achieving good agreement of model and measurement for a test layer of red pigment in resin (Figure 4). This procedure has been applied to all pigments used in our work.

Radiation transport in paper is an important contribution to the optical properties of prints. In our model we use certain volume fractions of scattering (e.g. air voids and chalk) and fluorescent particles. As an example the simulated spatial reflection (point spread function) of the paper layer shown in Figure 1 is shown in Figure 5.

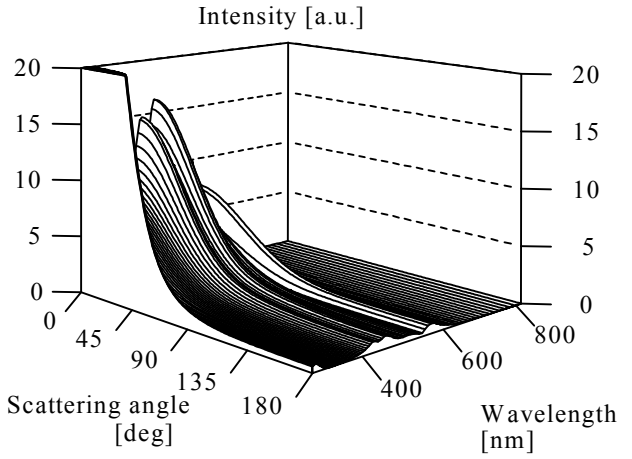

Figure 3. Angular dependence of the scattering of a red pigment, as obtained from Mie theory.

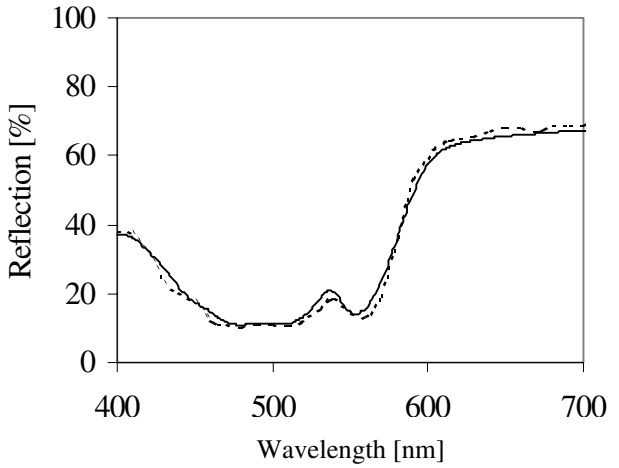

Figure 4. Measured (solid line) and simulated (dashed) reflectance of a red pigment layer on an aluminum mirror.

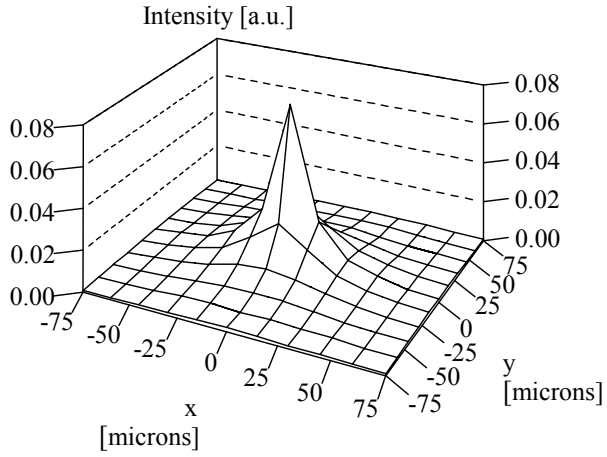

Figure 5. Example of simulated light spreading in paper for a chalk content of 3%. A collimated light beam is incident in the center (x=0, y=0). The graph shows the spatial intensity distribution of the emerging radiation on the top side of the paper.

To emphasize the lateral scattering features of our model, the reflection is simulated using different volume fractions of scattering particles. The result is shown in Figure 6. The increase in scattering particles has the expected effect on spatial reflection: Stronger scattering (realized by a higher chalk content in the paper) leads to a more localized point spread function. Both the lateral scattering as the fluorescence are features which are not adressable using the Kubelka-Munk method.

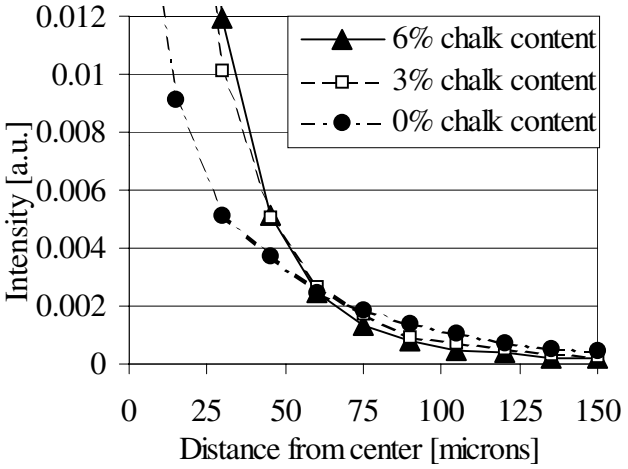

Figure 6. Point spread functions for different amounts of chalk in our paper model.

Printed Samples

From the results shown in Figure 6 it is expected that optical dot gain will be a natural outcome of the model. To investigate this, a black square is printed. A (microscope) picture is taken from the paper-toner transition (see Figure 7a). From the RGB image the Green values are taken (which scale with lightness). The average Green value is given in Figure 7a. Here the optical dot gain effect is clearly visible. This same effect is modelled using a model sample of similar shape as in Figure 7a. The reflection at 560 nm is simulated, and the average values are shown in Figure 7 b.

The absolute values of the measurement can not be compared with the simulation in Figure 7, because of the necessary differences in measurement set-up. From the relative values the correspondence in the optical dot gain effect is evident. In our described method, no scaling parameter is used like in the Yule-Nielsen approach: the dot gain effect is due to the actual scattering properties of the model paper.

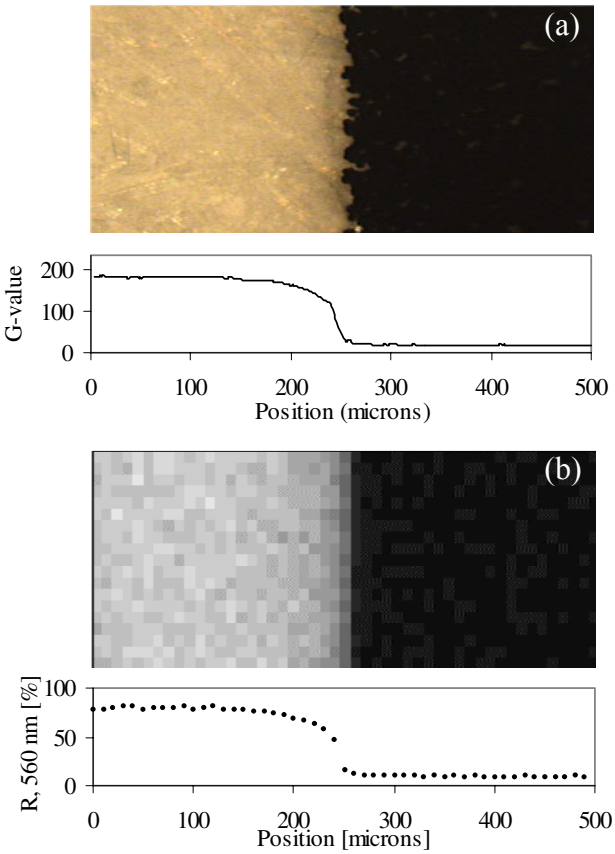

Figure 7 (a) Microscope picture (10x enlarged) of a toner-paper transition, with the measured spation reflection. (b) Simulated reflection at 560 nm of a model toner-paper transition, with the simulated spatial reflection.

Finally, test patterns are made consisting of line patterns with various coverages and frequencies. These patterns are both printed with black toner, and modelled. In the modelled pattern, the mechanical dot gain effect of the toner on paper is accounted for. The reflection values of the test patterns are measured and simulated. The resulting tristimulus Y-values (according to CIEXYZ, 1931, D65, 2° observer) are compared, as shown in Figure 8. Because specific test patterns are used instead of halftone patterns, the curve has a bend that deviates from the normal shape when a halftone pattern is used.

The result shown in Figure 8 indicates that our simulation approach is applicable to real halftoned images instead of line test patterns. If we use single or multi colored halftone patterns, the spectral approach of our method will make spectral color prediction of those patches possible.

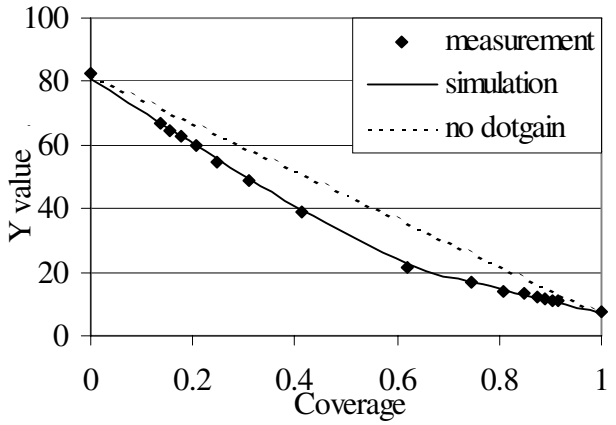

Figure 8. Y-values of a series of printed and simulated lined patches with increasing coverage. By the deviation from the straight line the influence of optical dot gain is visible.

Evaluation

An overview of the capabilities of our model in relation to already available models is presented in Table I. Most of the items in Table I are already mentioned in this paper. A few additional comments are given.

Although the available methods of color prediction can be succesfully applied in particular cases, they can not be used for all the factors that influence the resulting color of a print. Our model exceeds the limitations of available models. Because of the physical approach no free scalable parameters need to be fitted, making it robust for different measurement arrangements. Since fluorescence is highly dependent on the measurement arrangement, this phenomenon is an exception. Optical effects like color changes due to different light sources are an outcome using our model, but as with all color prediction models physical-chemical interaction like fluorescence quenching can not be simulated. Our approach is capable of handling geometric influences like smooth or rough surfaces. Using the model this will lead to glossy or diffuse surface reflections. Because of the flexible implementation of scattering in our method, we have the possibility to handle not only anistropic scattering, but also other complex scatterers like metallic or pearlescent scattering.

Our approach can be used to simulate the reflection of complex halftoned samples, but due to the ray tracing our computation times are a drawback. The computation of a full spectrum of toner on paper typically takes a few minutes on a modern PC.

Table I. Comparison Between Color Prediction Models

Applicability	*TvO*	**KM**	**YN**	**E**
Relate optical behaviour of toner ingredients with color of print	✓	-	-	-
Relate color with concentration and layer thinkness	✓	✓	-	✓
No use of free scalable parameters	✓	-	-	-
Independent of non-fluorescent experimental setup	✓	-	-	-
Independent of fluorescent experimental setup	-	-	-	-
Influence of surface roughness	✓	-	-	-
Lateral scattering	✓	-	-	✓
An-isotropic scattering	✓	-	-	-
Metallic or pearlescent pigments	✓	-	-	-
Dot gain	✓	-	✓	✓
Color prediction of halftoned multi-colored patches	✓	-	-	✓
Computational effort	High	Low	Low	(?)

TvO: this work
KM: Kubelka-Munk
YN: Yule-Nielsen
E: Emmel et al.

Conclusions

We have developed a new spectral color prediction model by advanced physical modelling of toner and paper. It is shown by thorough validation that the model corresponds well with experiments. Because of the generality of our approach, other color systems like ink or paint can be modelled in a similar manner.

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Biography

Gerben van Oosterhout received his Masters Degree in Physics from the Eindhoven University of Technology, the Netherlands, in 2000. Since then he has been working at Océ Technologies B.V., in the Research and Development laboratory. In cooperation with Wolfgang Theiss he is working in the field of color prediction modelling. Furthermore, he is active in the fields of optics and illumination of color scanning.