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Implementation of the four-flux model for spectral and color prediction of 2.5D prints

Théo Phan Van Song[1,2], Christine Andraud[2], Maria V. Ortiz Segovia[1]; [1]Océ Print Logic Techonolgies SA, Créteil, France; [2]Centre de Recherche sur la Conservation des Collections (CRC), MNHN, Paris, France

Abstract

Optical models to predict visual appearance of 2D prints are relatively well-known. Two-flux models, such as the Kubelka-Munk (KM) theory, are the most commonly used and offer good prediction rates. However, most two-flux models assume that the ink layer and the printing support have the same optical indices neglecting their wavelength dependency. An improvement of such constraint would be to include detailed optical indices of the inks in current models. In this paper we compute optical indices of our inks by printing ink stacks of different thicknesses on a transparent support for reflectance and transmittance measurements. Since KM-based models work under limited conditions, we input our computed indices into a more robust model. By taking additional fluxes into account, one can address the limitations of the two-flux approaches. For instance, the four-flux model considers two collimated and two diffuse fluxes propagating upward and downward the layer stack offering better reflectance and transmittance predictions especially when translucent materials are involved. Our four-flux theory including inks optical indices enables us to make spectral predictions of 2.5D prints without any preliminary measurements. The model is fairly accurate with primary colorants since the ΔE_{94} *values do not exceed 1 unit.*

Introduction

The advent of 2.5D and 3D printing technologies has increased the need to control print properties such as color, glossiness, translucency, and texture [1-2]. In the case of UV curable inks and varnishes, one can print not only on paper, metal and glass but also on top of a cured layer of the same ink. This characteristic makes UV inks suitable for what we refer as 2.5D printing, on which several inkjet layers of ink are piled up until a desired surface is achieved. The ability to control the printout roughness as well as the use of translucent materials creates exciting prospects for the printing of glossy and/or translucent textured surfaces.

In the printing industry, color management is mainly based on ICC profiles. These sets of data are established via a mathematical treatment of colors measured with a tri-stimulus colorimeter or a spectrophotometer on a printed color chart. Yet, by considering the physical properties of a printed surface, the optical approach would be actually much more beneficial for a simple and accurate color management. It would require modeling the multiple reflections and scattering of light at the interfaces and inside the media composing the material. For stacks of planar layers, such as printed surfaces, one can solve the radiative transfer equation (RTE) [3]. Radiative transfer models are appropriate to predict optical properties of heterogeneous materials consisting of particles dispersed in a matrix. To that end, a layer of ink can be modeled as pigments inside a binder. The RTE takes into account the orientations of the incident and scattered fluxes. When only two hemispherical diffuse fluxes are considered, the RTE has analytical solutions directly linked with the reflectance and the transmittance factors, known as the Kubelka-Munk (KM) formulas [4-6].

This two-flux model and its extensions are the most commonly used because of their simplicity [7]. They offer good prediction rates provided that strict conditions of the two-flux approach are satisfied (i.e. Lambertian illumination, optically thick films, highly scattering and weakly absorbing particles). However, the two-flux theory fails when the illumination is collimated or when dealing with translucent layers [8], like the ones produced with a 2.5D printer. Two-flux models also require macroscopic measurement of the reflectance and transmittance of one component for further predictions. Most of these problems can be solved with a moderately more complex four-flux model [9-11]. With two additional collimated fluxes, the four-flux model improves the spectral predictions when the illumination or a part of it is collimated.

Moreover, KM-based models used for color prediction have assumed until now that the ink layer and the printing support had the same refractive index, generally 1.5, to compute the reflection at the ink-air interface. Not only these models omit the wavelength dependency of the refractive index but they also neglect the part of light that is attenuated by overlooking the imaginary part of the complex refractive index. An improvement on such constraints would be to include detailed optical indices of the inks. Unfortunately, the refractive index *n* and the absorption index *k* are usually unknown for the complete spectrum and obtaining them is not an easy task [12]. Computing inks optical indices is possible by printing ink stacks of different thicknesses on a transparent support for reflectance and transmittance measurements. These approximate indices have shown to ameliorate prediction of some underlying physical phenomena that affects the color rendering of prints such as the bronzing effect [13].

In this work we compute our ink optical indices to include them into a multilayer four-flux matrix radiative transfer model as proposed by [10]. We start by presenting the four-flux model without explicitly focusing on the resolution of the RTE. Then we briefly explain how the inks optical indices were computed and incorporated into our model along with the others parameters. The spectral properties of flat relief samples of primary colorants (CMYKWV) at different thicknesses are computed by this model that accounts for the different optical components (i.e. interfaces, ink layer and substrate). We assume that pigments inside the ink layer are spherical scatterers with a given size distribution and concentration. Lastly, our four-flux model simulations are compared to spectroscopic measures. By using the CIELAB ΔE_{94} color distance metric, we can assess our model by quantifying the deviation between the measured and the predicted color spectra.

Radiative transfer four-flux model incorporating inks optical indices

Four-flux model to solve the radiative transfer equation (RTE) in an ink layer

One full tone sample of ink is modeled as a layer of thickness d containing a small concentration c of pigments (scatterers). We consider pigments as spherical scatterers. Lorenz-Mie theory tells us that when light hits a spherical particle, it interacts on the extinction cross section which represents the surface of light lost from the incident beam due to absorption and scattering. The extinction cross section C_{ext} is therefore defined as the sum of the absorption and scattering cross sections C_{abs} and C_{sca} which depend on the size and the optical indices of the scatterers. The scattering phase function gives the angular distribution of scattered light and depends strongly on the size of the scatterers. In the Rayleigh model, the scattering would be quasi-isotropic. But the bigger the particle, the more anisotropic and forwardly oriented the scattering is.

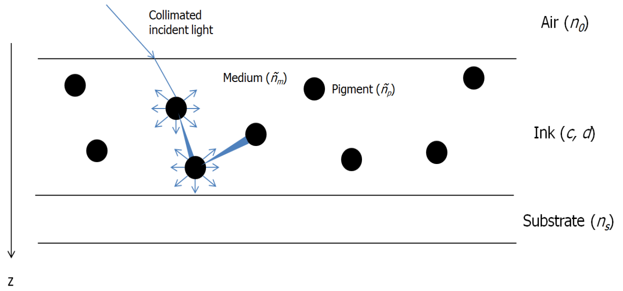

Figure 1. *Incoherent multiple scattering inside an ink layer under collimated illumination.*

Mie theory [14] allows one to compute how much light is absorbed and scattered by a single spherical particle. In the case of an ink layer (i.e. an absorbing and scattering medium), made of a batch of identical particles, multiple scattering prevails because the length travelled by light is higher than the particle's extinction mean free path. In other words, incident light interacts with more than one particle before leaving the medium (see Figure 1). Furthermore, pigments are assumed to be randomly distributed which induces an incoherent scattering. Considering those scatterers as spherical particles and their concentration low in the medium, it is possible to establish the sum of the light beams inside the medium. This leads to the RTE [3]. As explained before, the four-flux approach as described by [9] is a simple solution to the RTE.

The four-flux model treats multiple scattering inside a parallel planar structure of material with a possible substrate and takes into account the optical interfaces between the surrounding medium (air) and the slab (ink), therefore reducing the RTE to a one dimension problem (Figure 2). The incident radiation can be either diffuse, collimated or both. The modeled radiation inside the stack of layers is composed of two collimated beams, I and J and two semi-isotropic diffuse beams i and j. I and i are propagating to positive z while J and j are propagating to negative z. The differential equations defining the four-flux model are:

$$\frac{dI}{dz} = -(K+S)I \tag{1}$$

$$\frac{dJ}{dz} = (K+S)J \tag{2}$$

$$\frac{di}{dz} = -(1-\zeta_c)SI - \zeta_c SJ + \varepsilon(1-\zeta_d)Sj - \varepsilon(1-\zeta_d)Si + \varepsilon Kj \tag{3}$$

$$\frac{dj}{dz} = \zeta_c SI + (1-\zeta_c)SJ - \varepsilon Ki - \varepsilon(1-\zeta_d)Si + \varepsilon(1-\zeta_d)Sj \tag{4}$$

where $K=\rho C_{abs}$ and $S=\rho C_{sca}$ are respectively the absorption and the scattering coefficients (ρ is the number of particles per volume unit). ζ_c and ζ_d are the forward scattering ratios for the collimated and diffuse beams respectively that depend on the scattering phase function. $(1-\zeta_c)$ and $(1-\zeta_d)$ are the backscattering ratios. ε is the average path-length parameter introduced by [9]. When the diffuse light crosses a length dz, the average path length which is traveled over is actually εdz. ε is equal to 1 for a collimated radiation and to 2 for a Lambertian radiation.

By integration of the system (1)-(4) with boundary conditions, the four-flux model computes reflectances R_{cc}, R_{cd}, R_{dd} and transmittances T_{cc}, T_{cd}, T_{dd} of the modeled ink slab (*cc* for collimated-collimated; *cd* for collimated-diffuse; *dd* for diffuse-diffuse).

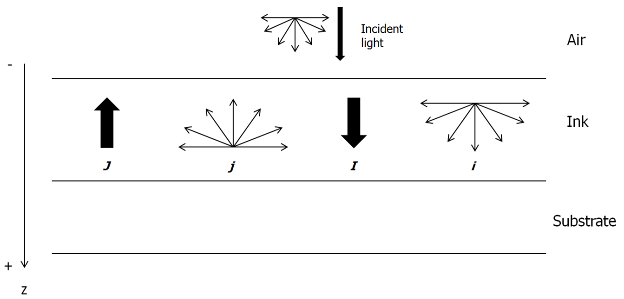

Figure 2. *Geometry of the four-flux model. Illumination can be diffuse and/or collimated. This approach models a radiation constituted of two collimated beams I and J and two diffuse fluxes i and j inside a plane parallel slab.*

Refractive index and absorption coefficient computation

A layer of ink can be seen as pigments of complex refractive index $\tilde{n}_p=n_p+ik_p$ randomly spread inside a medium of complex refractive index $\tilde{n}_m=n_m+ik_m$. The real parts n_p, n_m are the refractive indices and the imaginary parts k_p, k_m are related to the transmittance of the ink layer according to Beer's law: $t_i = e^{-\alpha h}$ where h is the thickness of the ink layer and α is the absorption coefficient: $\alpha=4\pi k/\lambda$.

Ellipsometry, based on polarization analysis, is considered the main technique for optical indices measurements. Nonetheless, it requires a very flat, homogenous and non-scattering sample. That is why this method would be inadequate for inks. Instead we use a method proposed by [13] based on a flux transfer model that relies on the multiple reflections and transmissions of light between the layers and interfaces. Such a method requires printing on a transparency film and computing the indices from reflectance and transmittance measurements.

Samples of every primary colorant were printed at different thicknesses using Océ 3D High Resolution Printing Technology. This technology allows accurate control of a print thickness h. We use the formulas from [13] to compute the indices from the reflectance and transmittance measurements. Computations account for the effect of the substrate. Results show that indices are clearly wavelength-dependent and that inks are also very absorbing in a certain waveband (see Figure 3). The results provide us an effective index for the ink.

However, our model requires two sets of indices, one for the medium and one the pigments. Thus, we use the computed indices as our pigment indices and the indices of a transparent ink, an ink without pigments, as our medium indices.

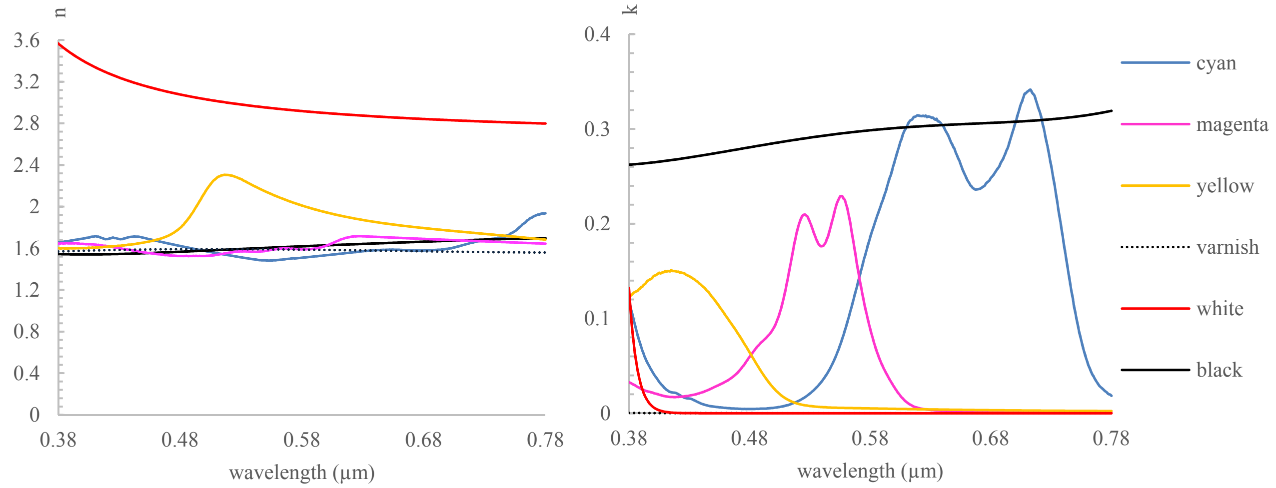

***Figure 3.** Real part (left) and imaginary part (right) of the complex refractive index of inks used by Océ 3D High Resolution multi-channel printer as a function of wavelength.*

Assessing the efficiency of the four-flux model to predict spectral properties of ink layers

Modeling ink layers using optical parameters

As explained before, this model considers a collimated illumination and is based on the Lorenz-Mie theory which takes into account the size of the pigments that compose a given ink. Pigment particles are grinded several times to ensure they are held in stable dispersion in the ink. The size distribution is typically D50: 100 to 150 nm and D95: 250 and 300nm. The model also considers the volume fraction of pigment in the ink (2 to 5%) and the layer thickness.

In this work, we model layers of all colorants used by the printer: cyan (C), magenta (M), yellow (Y), black (K), white (W) and varnish (V) were printed independently in superposition from one to five layers (which correspond to a thickness of about 9 to 45 µm) without any substrate. All layers have 100% ink surface coverage.

For each colorant, we set a pigment size distribution, a volume fraction of pigment and the previously computed optical indices of both the medium and the pigments. Therefore, for each colorant, we carry out five simulations where only the thickness of the simulated ink slab varies.

Then, our model calculates the absorption (C_{abs}) and scattering (C_{sca}) cross-sections (and so the absorption and scattering coefficients K and S) as well as the forward scattering ratios ζ_c and ζ_d for each wavelength from 0.38 to 0.78 µm. Ultimately, the matrices of the four-flux model lead us to R_{cc}, R_{cd}, T_{cc} and T_{cd}. Given that our simulations consider no diffuse component in the illumination, R_{dd} and T_{dd} are zero.

Typical color prediction models require the measurement of the reflectance and transmittance of at least one component to predict the reflectance and transmittance of stacks of similar components. On the other hand, our model relies on the radiative transfer theory computed through the intrinsic characteristics of the inks, using as inputs their optical indices. However, we have presented here a set of spectral measurements that allowed us to characterize our inks and compute their optical indices, but that were no required by the model per se. This means that if the ink maker provides the ink indices, the model can be used directly with no need of further measurements.

Simulations vs measurements

Samples were printed on a slippery surface which enables us to remove the ink slab off the substrate. This facilitated reflectance and transmittance measurements without any substrate to compare the measured spectra with our model computations. Measures were made using a CARY 5000 Agilent with an integrating sphere capable of measuring in both specular included and specular excluded modes.

Figure 4 displays the results of the model computations and the spectro-photometer measures of all the inks (from top to bottom C, M, Y, K, W and V). The left column gathers the reflectance spectra and the right column the transmittance spectra. The solid black lines correspond to the measured spectra in specular included mode while the dashed red lines correspond to the predicted spectra. The predicted spectra are the sum of the collimated-collimated component and the collimated-diffuse component (i.e. displayed predicted reflectance is $R_{cc} + R_{cd}$ and displayed predicted transmittance is $T_{cc} + T_{cd}$).

For all inks, the transmittance depends heavily of the number of layers as it progressively decreases as the thickness increases. On the other hand, the reflectance is not as much thickness-dependent but it still increases with the thickness in the more scattering regions of each colorant (notice it more clearly in the yellow and the white cases). To assess the deviation between the predicted and measured spectra, we use the CIELAB ΔE_{94} color distance metric. Colorimetric coordinates were calculated from predicted and measured reflectance and transmittance spectra using the CIE-XYZ convention with a D65 illuminant for the 2° standard observer then converted into CIELAB coordinates.

A summary of the predictions can be found in Table 1.

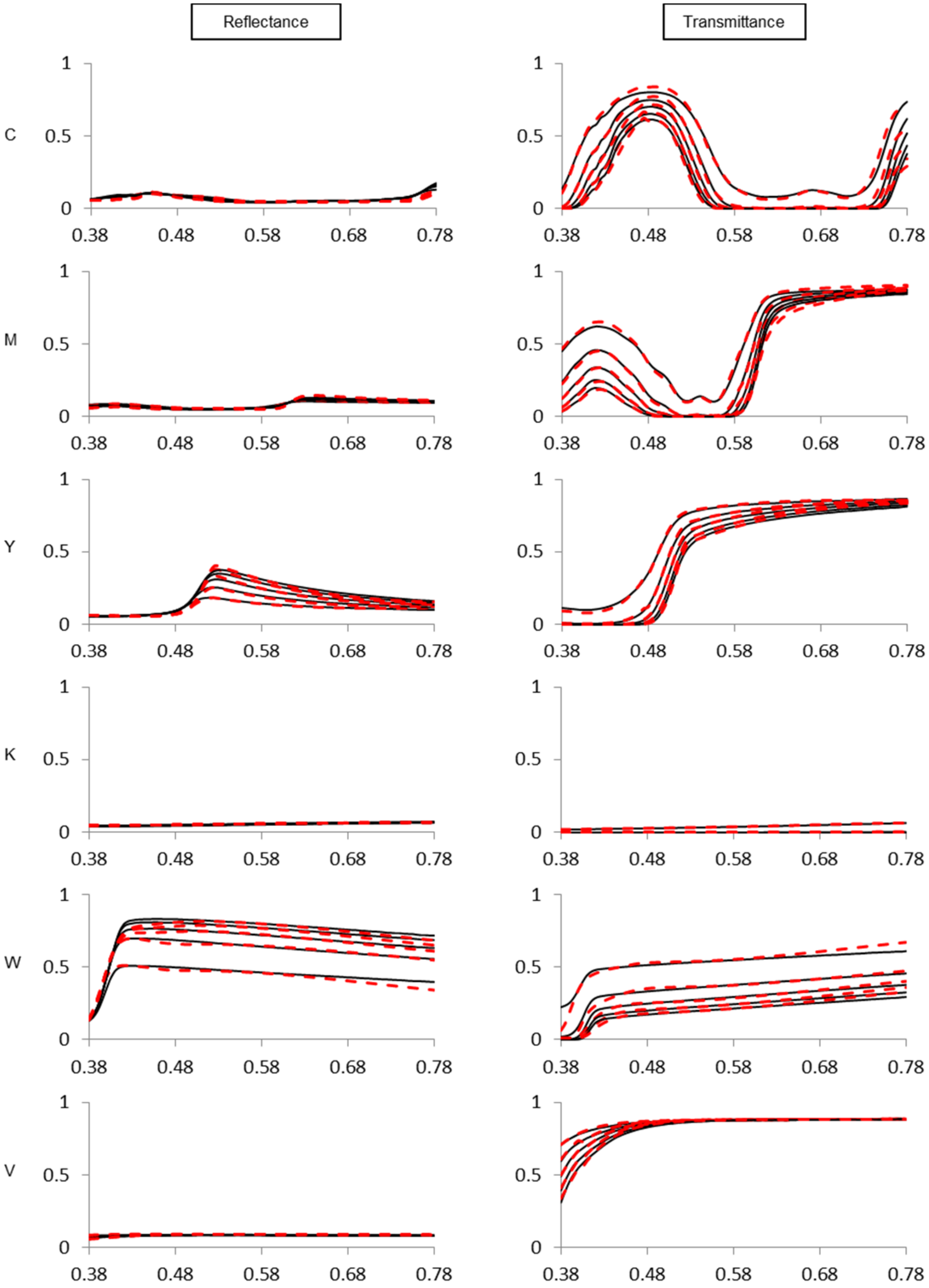

Figure 4. *Predicted (red dashed line) and measured (black solid line) reflectances (left column) and transmittances (right column) of full tone samples of C, M, Y, K, W and V for layers of different thicknesses (9 to 45 µm).*

Table 1: Evaluation of the color prediction of fulltone colorants printed with different thicknesses using CIELAB ΔE_{94}.

		Cyan	Magenta	Yellow	Black	White	Varnish	Aggregate
Reflectance	mean ΔE_{94}	0.81	0.65	0.92	0.89	0.98	0.83	0.85
Transmittance	mean ΔE_{94}	0.95	0.91	0.39	0.31	0.79	0.46	0.64

Predictions are fairly accurate standing below 1 CIELAB ΔE_{94} unit. Transmittance predictions, which notably depend on absorption, are satisfying overall and prove that the calculated absorption coefficients are accurate. Reflectance predictions are also satisfying. Color differences are higher for yellow and white which are the two most scattering colorants. This indicates that our predictions are highly dependent of the refractive index. The computed indices prove to be precise enough for inks with small scattering regions but are less reliable for strongly scattering layers. The computation of one component's refractive index over the whole spectrum is troublesome with spectroscopic measurements. Better measurements and calculation will enhance prediction performances.

Conclusion

Controlling the main four aspects describing the visual appearance of a print (color, gloss, translucency and texture) has become even more significant with recent advances in 3D printing technologies and the addition of an extra dimension. Color prediction models such as KM-based models have shown good accuracy but are limited in a number of ways. In this work, we characterized inks by calculating their refractive index real and imaginary parts. Using a radiative transfer four-flux matrix model, we took these optical properties into account by modeling an ink layer as a heterogeneous material consisting of pigments dispersed in a medium.

Our model computes both the transmittance and the reflectance of a print sample with non-zero height without any preliminary macroscopic measurement. Here we modeled layers of ink with no substrate and achieved good prediction accuracy. Yet, we can still improve these predictions. Our model depends heavily on the ink characteristics and optical indices. This was expected as we deduce the refractive index and absorption coefficient from spectroscopic measurements by using a flux transfer model. Accordingly, inaccuracies can be introduced since the computation of the inks complex refractive index is reliant to the measurement environment. Not only the use of exact optical indices but also the fine tuning of other model parameters (i.e. pigment size and pigment concentration) will improve predictions. The next step is to evaluate whether our model can compute the reflectance and transmittance of ink mixtures (such as red (magenta + yellow), green (cyan + yellow) and blue (cyan+ magenta)) where the primary colorants take equal and non-equal parts. On the long term, by characterizing the spectral properties of inks and substrates, this model could predict any color on any substrate under different illuminations without any preliminary macroscopic measurement. It could also address the inverse problem: compute the quantities of ink needed to achieve a targeted color under a given illumination and observation conditions.

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Author Biography

Théo Phan Van Song received his master's degree of engineering from the Institut National des Sciences Appliquées de Rennes in 2015. He is currently preparing a PhD on the subject of relief prints at the Muséum National d'Histoire Naturelle of Paris within the CRCC (Centre de Recherche sur la Conservation des Collections) in collaboration with Océ Print Logic Technologies.