# Spectral predictions of rough ink layers using a four-flux model

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## Abstract

*Predicting how light propagates through a stack of ink layers for spectral reproduction is a challenge only optical models can face. In particular, the four-flux model offers directional information about the part of light specularly reflected and transmitted and the part of light scattered in other directions. The surface roughness influences strongly the ratios of collimated and diffused light. In this paper, we describe how a radiative transfer four-flux matrix model can account for rough interfaces and show how roughness impacts the measured components of the reflectance and the transmittance of stacks of ink printed with different textures. The measurements are then compared to computations of the model with colorimetric and spectral metrics. Results are encouraging, considering that the predictions are made without any measurements directly inputted into the model, with the median color difference mostly below 2 $\Delta E_{94}$ units for total reflectance and transmittance whatever the roughness.*

## Introduction

Visual appearance is the most crucial criterion affecting customer preference in the graphic arts industry. To guarantee consistency and harmony, it needs to be meticulously managed. In the printing industry, appearance has long been assimilated to color. Conversely many objects have a more complex outward aspect and the CIE have identified four headings to characterize visual appearance: color, gloss, translucency and texture [1].

The development of 2.5D and 3D digital printers is an exciting prospect as these systems are expected to manage these four characteristics. 2.5D printing, as we understand it here, is a technique where multiple layers of ink can be piled up at a desired location. By manipulating the inks, gloss and texture can be managed through the controlled printout roughness [2] while relief can be produced [3]. Varnish can also be applied to the surface topology to render matte or shiny aspects [4]. Finally, translucency can be adjusted by taking advantage of the opacity of the inks from the opaque white ink to the clear varnish [5].

The color rendering of a printed surface depends on many parameters such as the color and texture of the print support or the translucency and viscosity of the inks. Meanwhile, the observation conditions and nature of the light illuminating the object affect the visual rendering. Generally, it's the broad range of potential interactions between ink, the print support and light that makes color management so complex in printing applications [6].

Methods based on physical models for spectral reproduction have been developed in recent years [7]. In particular, flux transfer matrix models can predict the spectral reflectance and transmittance of prints and stack of prints. Two-flux models [8] including the well-known Kubelka-Munk formulas [9] are often favored because of their efficiency and simplicity.

However inks are transparent substances and two-flux models don't work well with translucent layers [10]. With 2.5D printing, we're able to stack identical or non-identical layers of ink. Transfer matrices are therefore appropriate to predict the spectral properties of our printed materials. Accordingly, we choose to use a four-flux model [11-12] with its matrix formalism [13] which is suited for a wider range of scenarios and offers directional information. We use a radiative transfer version of the model like in [14] which consists in modeling the single scattering by a particle and then computing the multiple scattering by considering stacks of layers [15].

In a previous work, we employed this four-flux model to characterize and simulate reflectance and transmittance spectra of our primary inks [16]. We then applied the same four-flux model for the color prediction of secondary colorants without preliminary macroscopic measurements [17]. These predictions were made for total reflectance and transmittance spectra (diffuse + collimated components) of stacks of fulltone ink layers (100% surface coverage) without any substrate. Moreover, we supposed the air/ink and ink/air interfaces were flat. However, perfectly plane interfaces exist only in ideal scenarios while the surface roughness influences the way light is reflected and transmitted.

In this paper, we show the impact of the surface roughness on the distribution of diffuse and collimated light in reflectance and transmittance. We also model rough stacks of ink and take advantage of the directional information offered by the four-flux model to make separate predictions of the collimated and diffuse components. In the first part, we first recall the basis of our model and highlight its advantages over other models. We also explain how rough interfaces are modeled to account for the texture and go towards appearance management. In the second part, we demonstrate how this surface roughness affects both the part of light that is regularly reflected and transmitted and the part scattered out of the specular directions. Finally, we present results of the model and discuss the comparisons between predictions and measures made with a spectrophotometer equipped with an integrating sphere for specular included and specular excluded values.

## Framework of the radiative transfer four-flux model

### *A microscopic approach*

Our model is a four-flux model [11] solving the radiative transfer equation (RTE) [18] by considering light going through the layer is made of two collimated ($I$ and $J$) and two diffuse fluxes ($i$ and $j$). The equations defining the model are:

$$\mathrm{dI/dz} = -(K+S)I \quad (1)$$
$$\mathrm{dJ/dz} = (K+S)J \quad (2)$$

$$\mathrm{di/dz} = -(1-\zeta_c)SI - \zeta_c SJ + \varepsilon(1-\zeta_d)Sj - \varepsilon(1-\zeta_d)Si + \varepsilon Kj \quad (3)$$
$$\mathrm{dj/dz} = \zeta_c SI + (1-\zeta_c)SJ - \varepsilon Ki - \varepsilon(1-\zeta_d)Si + \varepsilon(1-\zeta_d)Sj \quad (4)$$

$K$ and $S$ are respectively the absorption and the scattering coefficients. $\zeta_c$ and $\zeta_d$ are the forward scattering ratios for the collimated and diffuse beams respectively. $(1-\zeta_c)$ and $(1-\zeta_d)$ are the backscattering ratios. $\varepsilon$ is the average path-length parameter introduced by [11]. When the diffuse light crosses a length $dz$, the average path length which is traveled over is actually $\varepsilon dz$. $\varepsilon$ is equal to 1 for a specular radiation and to 2 for a diffuse radiation.

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

Our radiative transfer model considers an ink is made of pigments randomly dispersed inside a binder. Our approach is therefore a microscopic one, antagonistic to the typical use of a macroscopic effective medium, and requires knowing precisely what an ink is. The main difference between our proposed model and previous color prediction models (CPMs) based on the two-flux theory rests on the computation of parameters $K$ and $S$. In two-flux model for color prediction of printed materials, $K$ and $S$ are computed with the very simple Kubelka-Munk formulas [9] hence the preliminary measurements of a macroscopic component usually made of ink printed on a diffusing support like paper.

In our model, we compute $K$ and $S$ differently, using $C_{abs}$ and $C_{sca}$, respectively the absorption and scattering cross-sections from the Lorenz-Mie theory [19].

In our case, $K = \rho C_{abs}$ and $S = \rho C_{sca}$ with $\rho = c/V$ the number of particles per volume unit [20], are intrinsic coefficients. $c$ is the volume fraction of pigment in the ink and $V = 4\pi r^3/3$ is the volume of the spherical pigment ($r$ is the radius of the particle). $C_{sca}$ and $C_{abs}$ are given by [21]:

$$C_{ext} = 2\pi k^{-2}\sum_{l=1}^{\infty}(2l+1)Re(a_l+b_l) \quad (5)$$
$$C_{sca} = 2\pi k^{-2}\sum_{l=1}^{\infty}(2l+1)(|a_l|^2+|b_l|^2) \quad (6)$$
$$C_{abs} = C_{ext} - C_{sca} \quad (7)$$

Here $k = 2\pi n_b/\lambda$ and $a_l$ and $b_l$ are Mie scattering coefficients (*Re* is for the real part), evaluated in terms of Ricatti-Bessel functions [22], which depend on the size parameter $x = kr$ and the relative index $m = n_p/n_b$ with $n_p$ and $n_b$ the refractive indices of the pigment and the binder respectively.

Therefore, the inputs of our model are the optical indices of the pigment and binder forming the ink as well as the pigment size and volume fraction in the ink. In other words, by retrieving the intrinsic characteristics of the inks, we can bypass preliminary measurements usually necessary for the computations of $K$ and $S$. Here we use the spectral characterization made in our previous work [16] based on the intrinsic attributes of the inks.

In KM-based models for printed materials, $K$ and $S$ are usually the coefficients of an effective medium (ink + substrate) while in our model, $K$ and $S$ are computed for the ink layer only. Inks are essentially translucent materials, which is why using a four-flux model is preferable. The differentiation between the ink and the substrate is a major step toward simpler calibration process for printers.

The substrate is also characterized by its optical indices. In the case where there's no print support (the ink can be printed on top of another layer of ink like in [16-17]), the substrate is air.

To sum up, our model has two main advantages over usual color prediction models. On one hand, because the inks and support are separately characterized beforehand, no preliminary measurements of macroscopic components are needed. On the other hand, it gives directional information on the amount of light that is reflected and transmitted. Since we consider that light is composed of two diffuse and two collimated fluxes, we can predict spectrally the collimated and diffuse components of both the reflectance and the transmittance.

## *Accounting for rough interfaces*

Because we distinguish the collimated and diffuse components, our model needs to account for rough interfaces that lead to surface scattering that we show in the next section. To model the surface roughness, we adopt a method based on the Kirchhoff theory and use the RMS heights σ for each interface. The attenuated collimated reflectance ($R'_{cc}$) and collimated transmittance ($T'_{cc}$) are defined by [23]:

$$R'_{cc} = R_{cc}\exp(-(4\pi\sigma n_1\cos i/\lambda)^2) \quad (8)$$
$$T'_{cc} = T_{cc}\exp(-(2\pi\sigma(n_1\cos i - n_2\cos t)/\lambda)^2) \quad (9)$$

In the case of a single ink layer without substrate, $n_1$ is the refractive index of the ink binder and $n_2$ the one of the air. $i$ and $t$ are respectfully the incident angle and the transmitted angle. $R_{cc}$ and $T_{cc}$ are the collimated-collimated reflectance and transmittance coefficients for a plane interface. Our model therefore accounts for the texture of each interface of the material as a function of illumination and viewing angles.

In that sense, our model falls within the framework of appearance management because it considers the roughness of the interfaces (texture) and it gives information not only about spectral reflectance (color) and transmittance (translucency), but also about specular reflectance at a specific angle (gloss). The interesting feature is that we can simulate these spectral data for any illumination angle assuming the incident light is collimated. Figure 1 illustrates the workflow of our model.

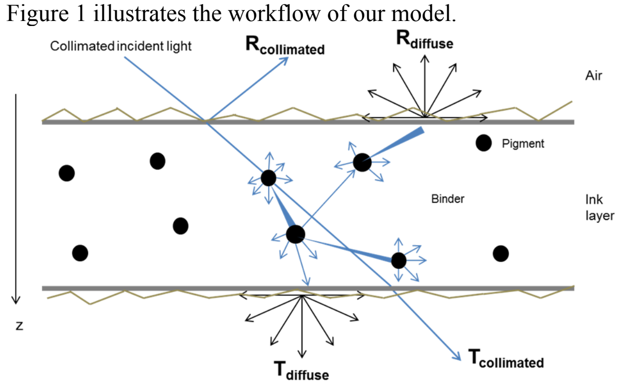


*Figure 1. Schematic representation of the workflow of the four-flux model: a layer of ink is illuminated by incident light (diffuse and/or collimated), light goes through the layer as a part is reflected specularly. Some part of light is directly transmitted while the rest interacts with pigments inside the layer which absorb and scatter light to render diffuse transmittance and reflectance. The model takes into account the roughness of the interfaces.*

## Spectral properties of rough ink layers

### *Measuring the impact of the surface roughness*

The roughness of an interface affects the surface scattering as rough surface attenuates both the collimated reflectance $R_{cc}$ and transmittance $T_{cc}$ (see equations (4) and (5)). In other words, some part of the collimated light in the case of a plane interface becomes diffuse with a rough interface. In the meanwhile, the total transmittance and the total reflectance supposedly remain the same whatever the roughness of the interface.

To demonstrate this phenomenon, we printed layers of cyan, magenta and yellow at different thicknesses (four different stacks for each ink with a thickness going from about 18 to about 45 µm). Each group of four stacks was printed with a different roughness. The surface roughness was controlled with the use of transparent varnish that doesn't impact the color and translucency of the stack. The first group is the rougher and was printed with no varnish; the second group is smoother as each stack was printed with one layer of varnish on top (about 10 µm); the third group has stacks printed with several layers of varnish on top (about 30 µm). The roughness of each group is illustrated in figure 2.

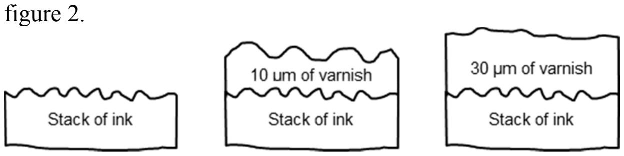


***Figure 2.*** *Illustration of the roughness of each printed group: from left to right, very rough surface, rough surface and smooth surface.*

We then measured the reflectance and transmittance of each stack. Measures were made using a CARY 5000 Agilent with an integrating sphere capable of measuring reflectance and transmittance spectra in both specular included (SCI) and specular excluded (SCE) modes at normal incidence. Measurements are done from 0.38 to 0.78 µm in steps of 0.005 µm under collimated light. Consequently, we are able to compare separately the directional components of the reflectance and the transmittance (collimated and diffuse) depending on the roughness.

Figure 3 displays these reflectance and transmittance measurements (total $t$, collimated-collimated $cc$, and collimated-diffuse $cd$) for stacks of a) cyan ink, b) magenta ink and c) yellow ink. The dashed blue spectra are the measurements of the very rough groups, the red solid spectra are the measurements of the second rough groups while the solid black spectra are the measurements on smooth groups.

The total transmittance $T_t$ is the same whatever the roughness for every ink at any thickness. Likewise, the total reflectance $R_t$ stays relatively steady. When the surface is smooth (black lines), the collimated transmittance $T_{cc}$ is at its maximum while the diffuse transmittance $T_{cd}$ is at its minimum. $T_{cd}$ increases with the roughness essentially in the scattering parts of each ink ([0.38-0.58] µm for cyan, [0.58-0.78] µm for magenta and [0.48-0.78] µm for yellow) while it mostly stays the same in the absorbing parts.

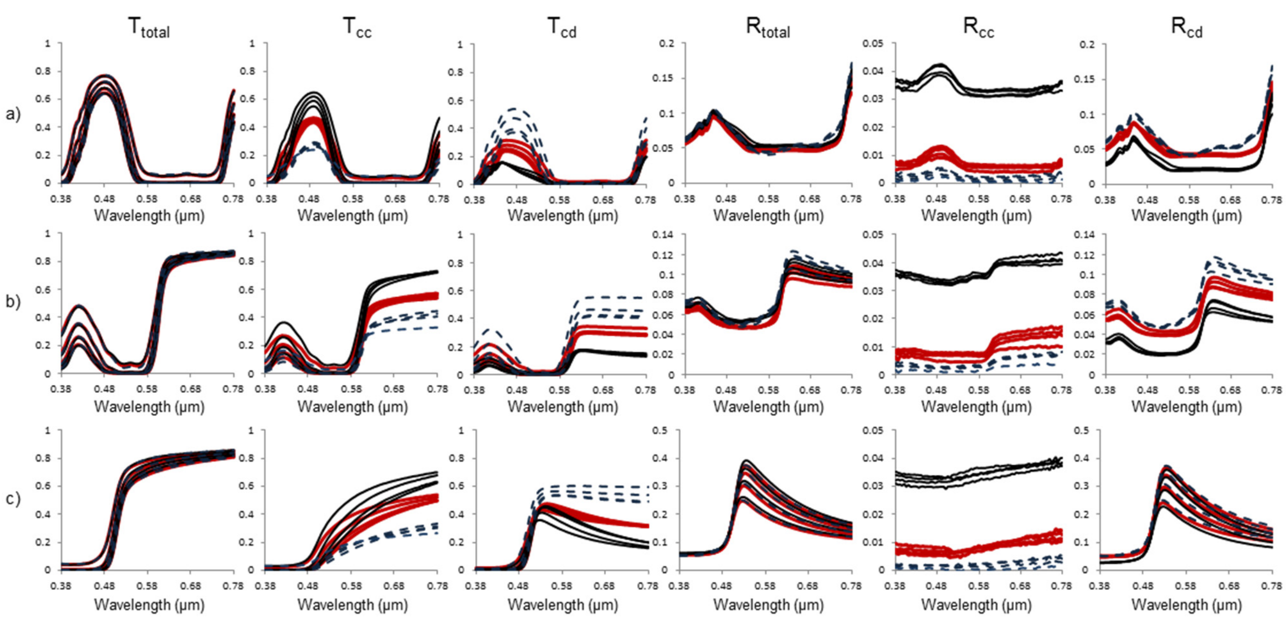


***Figure 3.*** *Total, collimated and diffuse transmittance, and total, collimated and diffuse reflectance measurements of four different stacks of printed layers of a) cyan, b) magenta, and c) yellow, with a thickness varying from about 18 to about 45 µm. Each group of stacks is printed with three different surface roughnesses: very rough (dashed blue lines), rough (solid red lines) and smooth (solid black lines). Measurements are made under collimated light at normal incidence.*

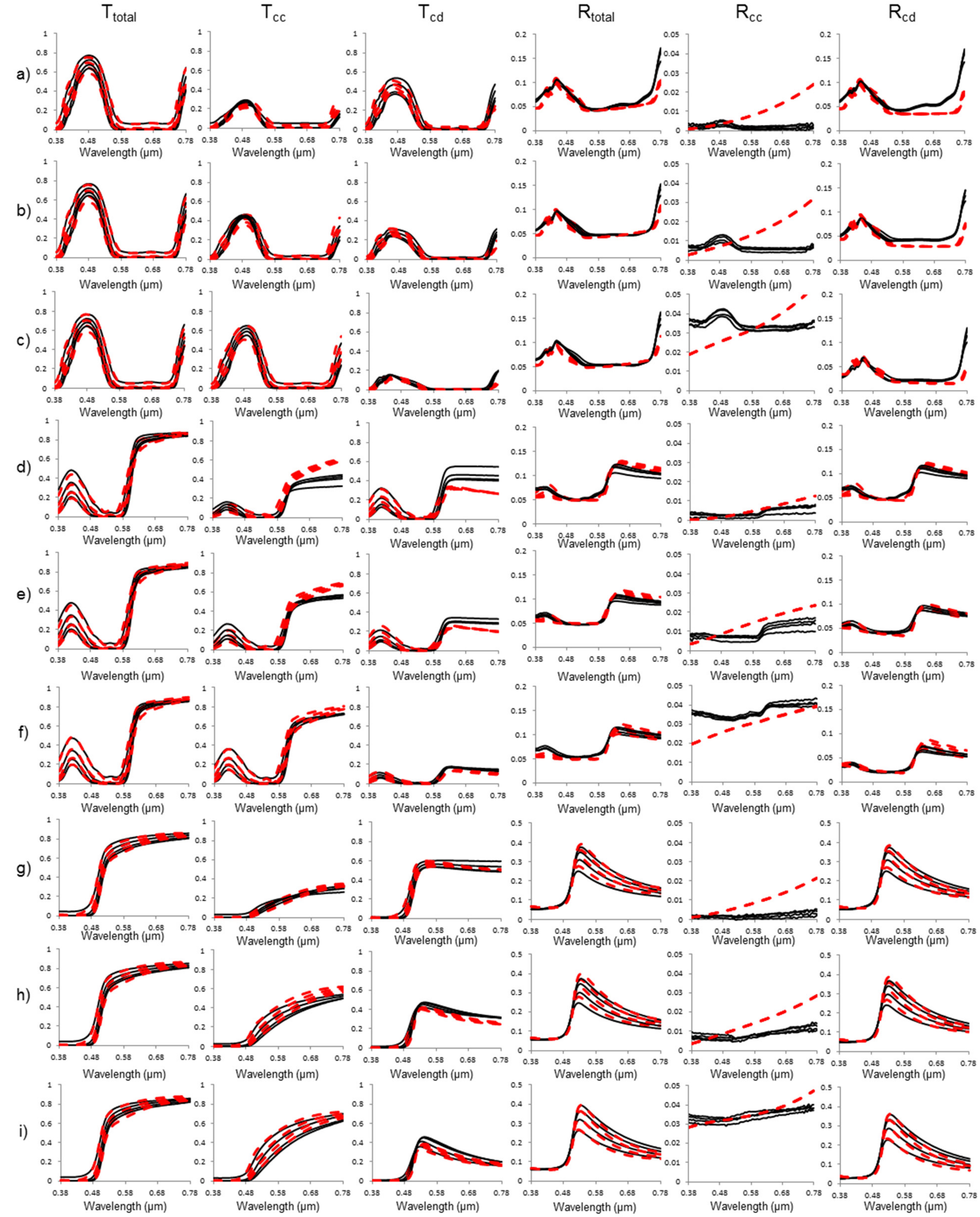


***Figure 4.*** *From left to right measured and predicted $T_{total}$, $T_{cc}$, $T_{cd}$, $R_{total}$, $R_{cc}$, $R_{cd}$ (cc=collimated-collimated, cd=collimated-diffuse) spectra of very rough, rough and smooth stacks of cyan (resp. a), b), c)), magenta (resp. d), e), f)) and yellow ink (resp. g), h), i)). Solid black lines are the measurements presented in figure 3 and dashed red lines are the predictions of the model.*

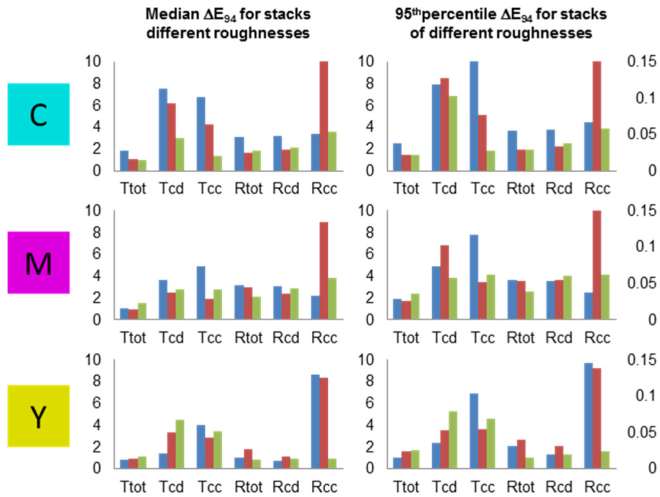


***Figure 5**. CIELAB ΔE94 color deviations and RMS deviations (RMSD) between the measured and predicted spectra (see figure 4) of stacks of cyan (top), magenta (middle) and yellow (bottom) ink printed with different roughnesses. The values here are the median and 95th percentile* $T_{tot}$, $T_{cd}$, $T_{cc}$, $R_{tot}$, $R_{cd}$, $R_{cc}$ *for each group of four stacks printed with different thicknesses.*

The reflectance has a similar behavior as the diffuse part $R_{cd}$ rises with rougher surface. However measurements show more of a vertical translation: collimated reflectance spectra $R_{cc}$ are just below 4% on the whole visible wavebands for smooth surface (similar to the value of reflectance at normal incidence of an interface between air and a material of refractive index n = 1.5) while it is almost reduced to zero with very rough surface. In fact, $R_{cc}$ is mainly due to the first reflection at the upper interface and should be achromatic as the reflection of the transparent ink binder. However a small coloration is noticeable in the measured spectra. This coloration is certainly due to the slight part of diffuse light going in the specular direction and into the spectrophotometer detector in SCI mode. Also $R_{cc}$ spectra are not exactly measured but deduced from the SCI and SCE measurements.

To assess the efficiency of our model and the way it handles rough interfaces, we modeled stacks of cyan, magenta and yellow at these different thicknesses and with three different roughnesses. Our aim here is to show that we can predict not only the total transmittance $T_t$ and total reflectance $R_t$ accurately but also the collimated $R_{cc}$ and $T_{cc}$ and diffuse $R_{cd}$ and $T_{cd}$ parts.

### *Results of the model predictions for different roughnesses*

The strength of our model is that no measurements are required as inputs. Only the previous characterization made for the primary inks [16] is necessary. To keep the calibration measurement-free, the surface roughness was not measured either. Several RMS heights values were tested empirically. A scaling of σ was established according to the model computation of $R_{cc}$. For very rough, rough and smooth interfaces, this parameter is respectfully equal to 0.1, 0.06 and 0.03 µm for the interface air/layer and 0.09, 0.05 and 0.03 µm for the second interface layer/air.

Figure 4 shows the predicted and measured spectra. The solid black lines represent the same measurements presented in figure 3 while the dashed red lines represent the model predictions. The median and 95th percentile color deviations (visual metric CIELAB ΔE94 computed from CIELAB color coordinates of the spectra using the standard illuminant D65) and spectral deviations (unweighted RMSD) between the measured and predicted spectra for each group of four printed stacks are presented in figure 5.

In general, we get a satisfactory accuracy for the predictions of $R_t$ and $T_t$ whatever the color and the thickness (mostly below 2 ΔE94 units). Conversely, the agreement is not that good between measured and predicted $T_{cc}$ and $T_{cd}$ spectra (especially for very rough and rough cyan stacks). Since the total transmittance is predicted accurately, this must be related to the distribution of the diffuse and collimated transmitted light. This can be fitted with a better roughness value at the exiting interface. However large deviations for $T_{cc}$ occur for the rougher stacks where $T_{cc}$ is at its lowest (see figure 4 a), d) and g)). Likewise, large deviations for $T_{cd}$ happen for the smoother stacks where $T_{cd}$ is considerably reduced (see figure 4 c), f) and i)).

Similarly to $R_t$, $R_{cd}$ predictions are close to the measurements with low RMSD while color differences are satisfactory. The biggest color deviations happen for the collimated-to-collimated reflectance $R_{cc}$. Predicted $R_{cc}$ spectra are independent of the thickness of the stack as they mostly depend on the reflection at the upper interface air/ink and the RMS heights value is constant for each group of four stacks. Equation (4) explains well the shape of the predicted spectra: at normal incidence $R'_{cc} \sim \exp(-(\lambda^{-1})^2)$. Therefore it is essentially attenuated for the smaller wavelengths. Yet the model is not to blame despite the high color differences because it has a physical reality: smooth glass of refractive index 1.5 has a collimated reflectance of 4% while rough glass presents reddish reflect. Also, these unacceptable color differences must be put into perspective with the very low RMSD for $R_{cc}$ especially for rough and very rough surfaces. Moreover, measured $R_{cc}$ were deduced from specular included and specular excluded measurements. As explained in the previous section, they also present a slight coloration that could come from the measurement technique.

Most predicted spectra are close to the measured ones according to RMSD values. When that's not the case, the visual perception is not necessarily impacted (for instance, $T_{cd}$ and $T_{cc}$ spectra for rough and very rough magenta stacks show high spectral differences but no so high color differences). Overall, the color deviation is more satisfactory for smooth stacks. That's in part due to the fact that the roughness parameter was set empirically and predictions for the smoother surface are a lot less dependent of this parameter. The model may also need to take into account the correlation length which is also important when describing surface roughness [23]. It's clear that there is a need to scale the RMS heights of the surface and more broadly characterize the roughness with not only the thickness and the ink printed, but also the size of the droplets of ink propelled onto the surface. Nevertheless these kinds of measurements are time-consuming and not essential for this study as our aim here is to show that the impact of the roughness on the nature of the light that is reflected and transmitted can be predicted. With a better knowledge and control of the surface texture, better predictions will come. Studies are currently underway at Océ [24].

Finally, it is interesting to notice how the transmittance and reflectance colors in the diffuse and specular directions can differ from one another. For example, the collimated transmittance of a stack of yellow ink is almost orange; its diffuse transmittance is yellowish while the reflectance is green (see spectra figure 4 i)). We could capitalize on these predictions for graphic arts applications such as multiview images that can show different images in different illumination conditions [25-26].

## Conclusion and perspectives

In this paper, we use a radiative transfer four-flux matrix model capable of predicting spectral properties of a stack of layers. The use of the four-flux model allows spectral predictions of the optical properties of translucent materials while the radiative transfer theory describes scattering within the material at a very small scale. Moreover, the four-flux model predicts separately the collimated and diffuse components of the reflectance and the transmittance.

The aim of this paper was to show how these components are connected to the surface roughness and how we can deal with the texture. The model presented is capable of predicting accurately the total reflectance and total transmittance of stacks of ink layer with different roughnesses. Predictions of the diffuse and collimated components with different roughnesses correlate with the measurements but are not always satisfactory in terms of color difference ($\Delta E_{94}$). Characterizing the surface roughness will improve the accuracy of the predictions. This work is currently performed by [24].

No preliminary measurements are inputted into the model to compute the reflectance and transmittance spectra of stacks of print and the inclusion of the surface roughness (the texture) is another step towards appearance management.

Future work for the model will consist in the separate spectral characterization of the print support or substrate. Until now, we considered the substrate to be air of refractive index 1. Other substrate might not be as easy to describe physically in terms of optical indices.

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