Next Generation Simulation Tools for Optical Properties in Paper and Print

Per Edström
Mid Sweden University, TFM, SE-87188 Härnösand, Sweden,
per.edstrom@miun.se

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Abstract

A large number of optical properties in paper and print are determined by measuring the light reflected from an illuminated paper surface. These measurements are interpreted through a model, and the one that has been in use in the paper industry since the 1930's (Kubelka-Munk) is deficient in some respects. This paper presents a selection of issues that will be in focus for future optical modeling, and shows what the next generation simulation tools may look like.

The anisotropy of the scattered light becomes increasingly important, and this will open up a large area of research that will both explain a number of outstanding issues and open for a new kind of material property design. Physically objective material parameters will be introduced instead of phenomenological model parameters. The wish to model the real structure of paper and printed paper products instead of homogenized approximations will drive the development of Monte Carlo models with greater explanative power, which in turn will give an increased need for characterization methods. Differences in optical standards between the paper and graphic arts industries will force harmonization or models for data exchange. The treatment of UV and fluorescence will be included in both light scattering simulation tools and color management tools, and there will be attempts of merging these two types of tools, which will open for another view on color reproduction. The directions of development outlined above are exemplified with recent results.

1. Introduction

A large number of optical properties in paper and print are determined by measuring the light reflected from an illuminated paper surface. These measurements are interpreted through a model, and the one that has been in use in the paper industry since the 1930’s (Kubelka-Munk) is deficient in some respects. Optical models are needed to design new paper products, to monitor the production process and in communication for trade purposes. Time raises new issues to tackle and higher accuracy is demanded, which drives the development of new models. This does not mean that Kubelka-Munk will be discarded. Rather, it will be complemented in areas where it does not suffice, and new areas will be opened.

1.1. Room for Improvement in Color Reproduction

One obvious use of optical models is in color reproduction for print on paper. It is well known that ordinary printing yields a gamut much smaller than what the eye can see. This is illustrated in figure 1, where the gamut of a typical print is contained within the largest viewable gamut. There is obviously still a lot of room for improvement. Optical models are needed to understand and control the color reproduction, and are important tools when trying to push the limits in this respect. This holds for the development of better top qualities as well as for lowering production costs.

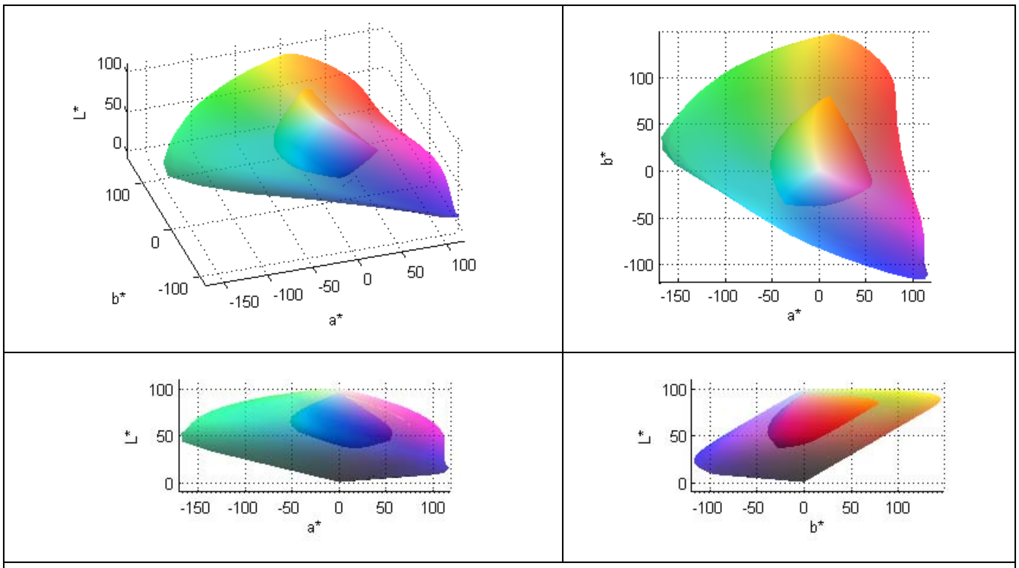

Figure 1. Color gamut of an ordinary print (inside) and the maximum gamut the eye can see (outside). There is obviously room for improvement, and the challenge is to move the inner gamut towards the outer in a controlled and preferably inexpensive way.

Optical modeling is moving forward at a high pace in these areas, and the solution of several outstanding issues is within reach. The next few years of research will generate tools and knowledge to extensively promote this development, and this paper presents some areas where advancement and new ideas can be expected to contribute.

1.2. Disposition of the Paper

This paper is divided in two parts. Section 2 presents a selection of issues that will be in focus for future optical modeling, and indicates the direction of development for the next generation simulation tools. Section 3 offers some examples of practical recent results on one of the outlined areas for future development, namely anisotropy, and can be considered as a sample preview of some unpublished results in that area.

2. Selected Issues in Future Optical Modeling and Next Generation Simulation Tools

2.1. Anisotropy and Goniophotometric Measurements

Most optical applications in the pulp and paper industry, in both measurement and modeling, implicitly rely on the fundamental assumption that the light distribution is perfectly diffuse. One example is instruments with d/0° geometry, where an integrating sphere is used to produce diffuse illumination. Another example is the ever-present Kubelka-Munk model [1-3] that is valid only for perfectly diffuse light. Both d/0° instrument geometry and the Kubelka-Munk model are prescribed by international standards [4-7] in the paper industry.

The assumption of a perfectly diffuse light distribution is not fulfilled in practice, however, and it has been shown that it is not fulfilled even in theoretically ideal situations [8-9]. This gives rise to errors in the interpretation of measurement data, and it causes anomalous effects in model output [10-15]. Several attempts have been made to explain [16-20] or correct for [21-22] such errors and anomalous effects, but these attempts have limited validity at the best.

Since in practice the light distribution is always more or less anisotropic (not perfectly diffuse), the way forward is to recognize and accommodate for this in models. Of course, there will always be broad situations where the effect of anisotropy, or the accuracy needed, is not larger than what can already be offered, and in such cases the models of today can still be used. However, models including anisotropy will enter the stage for several reasons, as briefly outlined below.

Demands on higher accuracy in optical measurements need to be met, and models used to interpret measurement data need to capture the real, non-ideal measurement situation, including the influence of the actual measurement geometry and the anisotropic reflectance from real samples. Some practical examples of this are given in section 3.

In order to handle the demand for objective material parameters and common optical methods and common standards for the paper and graphic arts industries (see sections 2.2 and 2.3 below), anisotropy needs to be accounted for.

Anisotropy can have a profound effect on the reflected light, and thus on the visual appearance of a sample. Understanding of the causes of anisotropy is a prerequisite to control the phenomenon. This in turn makes it possible to use anisotropy in optical design of new paper grades or new printed paper products. This includes angular dependent whiteness and color appearance, but also effects on opacity. Knowledge on such matters will give competitive advantages.

The angular distribution of scattered light can be quantified with a parameter called the asymmetry factor, which is a third optical parameter in addition to the scattering and absorption parameters. Knowledge on numerical values of the asymmetry factor for different materials is scarce, but is growing in other areas of research such as medicine.

Spectrally resolved goniophotometric measurements will come to use in a much larger extent to characterize the different constituent materials in paper and print with respect to anisotropy using the asymmetry factor. Angle-resolved models are needed to interpret such measurements. Angle-resolved models and measurement devices already exist that can handle the above, but standards are lacking. Basic research and industrially applied issues will together move this area forward, and industrial solutions are only a few years away.

2.2. Objective Material Parameters

Most models of today use phenomenological and model-dependent parameters, and this has some disadvantages. Since the parameters are not physically objective, they are not necessarily exchangeable between situations. Measuring the same samples with different instruments may give not only different values but also different ranking, which is not satisfactory. One example of this is estimation of optical properties from measurements using d/0° and 45°/0° geometry. Also, phenomena that might be considered physically linear do not necessarily appear so since the phenomenological parameters are not the actual physical quantities. This also diminishes the explanative power of the models, since the parameters are actually defined inside and by the models and therefore have no absolute and objective meaning outside.

It is therefore desirable to use physically objective material parameters, real paper properties and real process parameters. This makes data more exchangeable since they are independent of model and measurement geometry. This also gives the models more explanative power, as they convey more of the physical reality. Recent research has for example studied the influence of paper properties on color reproduction [23-24].

It is a clear trend that any new optical models introduced will need to use physically objective material parameters instead of phenomenological model parameters. Two types of optical models are finding their way into broader use in the pulp and paper industry, radiative transfer based and Monte Carlo based models, see figure 2, and both types do use physically objective material parameters.

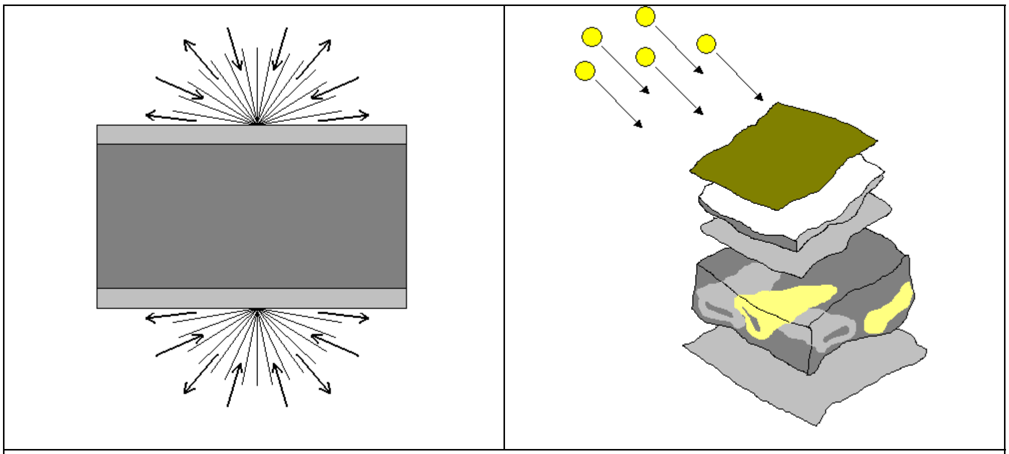

Figure 2. A radiative transfer model (left) considers the sample as a layered continuum, just like Kubelka-Munk, but is angle resolved and can therefore handle anisotropy. A Monte Carlo model (right) considers the actual structure of the model, but is slower and needs more parameters. Both model types use objective material parameters, which Kubelka-Munk does not.

The wish to model the real structure of paper and printed paper products instead of homogenized approximations will drive the development of Monte Carlo models with real explanative power, which in turn will give an increased need for characterization methods. Mid Sweden University will be launching an Open Source platform for Monte Carlo simulations of light scattering in paper and print (infrastructure is planned for autumn 2008 and first free code spring 2009), where it will be free to contribute and share computer code and structure data. Access to objective material parameters is essential for that initiative.

2.3. *Common Optical Methods and Standards for Paper and Graphic Arts Industries*

Methods and standards for measuring and handling optical properties differ between the paper and graphic arts industries. This is due to the fact that development over the years has been in relative isolation between the industries, with different issues and goals in mind. There are, among others, differences in measurement geometry (basically d/0° and 45°/0°) and in UV contents in the illumination. This gives samples different values and different ranking, and causes color failure. This is a hindrance for efficient data exchange and swift communication of optical properties between the industries, and it lowers production efficiency and causes waste. These issues are of great importance to handle, and a broad consortium has been formed that has formulated and submitted an application to the EU seventh framework program. No matter if that specific application is granted, cooperative research will move in this direction.

2.3.1. Handling the Geometry Issue

While introduction of and agreement on new common standards may be time consuming and expensive, more accurate interpretation of measurement data with better models may give accurate and efficient exchange of optical properties and specifications already from the different d/0° and 45°/0° measurement geometries of today.

Work in this direction is underway, and the necessary foundation in terms of knowledge and models already exists. Angle-resolved radiative transfer models have resolved parts of this issue [8-9], and have the potential to go to the bottom of it in the next few years of research.

2.3.2. Handling the Fluorescence Issue

The differences in UV content between the paper and graphic arts industries, the presence of OBA/FWA in paper, and the UV blocking effect of inks give rise to problems. This includes misunderstandings regarding paper whiteness and shade, proof-to-print mismatch and color failure, all resulting in waste and reduced production efficiency.

Solving this issue on the modeling side is feasible today, but will require a period of quantitative analysis and of finding efficient workflows in practice. The latter includes agreement on a common way to include UV and fluorescence in measurements. On the quantitative side, UV and fluorescence is already included in some light scattering simulation tools while others are under development, but the complicated chemistry involved and the effect on quantum yield needs more research. UV and fluorescence also needs to be included in color management and

ICC profile generation tools. The latter will need more research, but there are already initiatives.

Somewhat later, there will probably be attempts of merging light scattering simulation tools and color management tools, in order to move further in this direction. This will open for another view on color management, that one might tentatively call model based color management, including profile tuning and eventually profile calculation.

2.4. Nanomaterials

On the more applied side, although models will be needed as well, is the investigation and utilization of nanomaterials. This follows the general trend in other sciences, but the paper and graphic arts industries will probably not be in the forefront of research. Instead, there will be numerous opportunities to follow up on new material knowledge from other areas of research. Since nanomaterials can have extreme properties, they can probably find use in both surface treatment and in inks. One recent example is the discovery that ordinary candle soot contains multicolor fluorescent carbon nanoparticles [25], and it would be interesting to see what use this could have for paper whiteness or special inks.

With the extreme properties follows the challenge to characterize nanomaterials. Characterization will be needed both optically (scattering and absorption parameters, asymmetry factor, fluorescence properties) and otherwise (position in paper structure, effect on other properties such as chemistry, etc). A not so desired effect of nanomaterials is that their small size can have hazardous effects, which also needs to be investigated. The great discoveries in this area will be done in other sciences over a long period of time, but exciting possibilities will open to the paper and graphic arts industries in the utilization of those discoveries.

3. Examples of Practical Recent Results on Anisotropy

Digital Printing Center at Mid Sweden University runs research projects covering all issues mentioned in sections 2.1 – 2.3. This section offers some examples of practical recent results on anisotropy, which can be considered as a sample preview of some unpublished results in that area.

3.1. Effects of Anisotropy on Interpretation of Measurement Data

Most optical applications in the pulp and paper industry, in both measurement and modeling, implicitly rely on the fundamental assumption that the light distribution is perfectly diffuse. This goes for both the d/0° instrument geometry and the Kubelka-Munk model that are prescribed by international standards in the paper industry [4-7]. Since in practice the light distribution is always more or less anisotropic (not perfectly diffuse), models need – in order to correctly interpret measurement data – to capture the real, non-ideal measurement situation, including the influence of the actual measurement geometry and the anisotropic reflectance from real samples.

Figure 3 illustrates the basic 45°/0° and d/0° measurement geometries. They have in common the detection in a narrow solid angle around the normal to the sample, and thereby the implicit assumption in the following Kubelka-Munk calculations that the reflected light has the same intensity in all directions. They differ in the illumination, where 45°/0° has directed incident light at 45° and d/0° has diffuse illumination apart from the gloss trap.

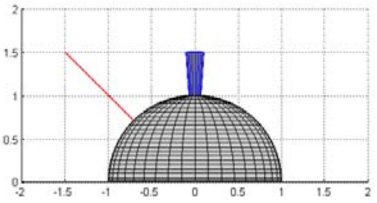

Figure 3a. Illumination (directed, red line) and detection (blue cone) in ***45°/0°*** *instrument geometry. Note that the device measures in the normal direction, and that following Kubelka-Munk calculations assume the grey half sphere as reflected intensity.*

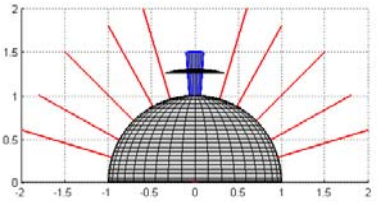

Figure 3b. Illumination (diffuse, red lines), detection (blue cone) and gloss trap (black) in ***d/0°*** *instrument geometry. Note that the device measures in the normal direction, and that following Kubelka-Munk calculations assume the grey half sphere as reflected intensity.*

Figure 4 shows how the intensity of the reflected light is actually distributed in an ideal measurement device of 45°/0° and d/0° type. As noted above, both instrument types measure in the normal direction only, and the following Kubelka-Munk calculations therefore assume a perfectly diffuse distribution (inner grey half sphere). It is obvious that this differs greatly from the actual distribution (outer white shape), and this yields errors even for the situation with perfectly isotropic single scattering that the system is designed for (topmost row). For a more anisotropic single scattering process the error increases, and in all cases is the total amount of reflected light underestimated. In the 45°/0° case, the highly asymmetric distribution should be noted, which obviously differs greatly from where Kubelka-Munk should be used. Although numerical values of asymmetry factor for paper are scarcely reported, it should be noted that values in the range 0.3 – 0.8 are common, which corresponds to the lower rows of figure 4.

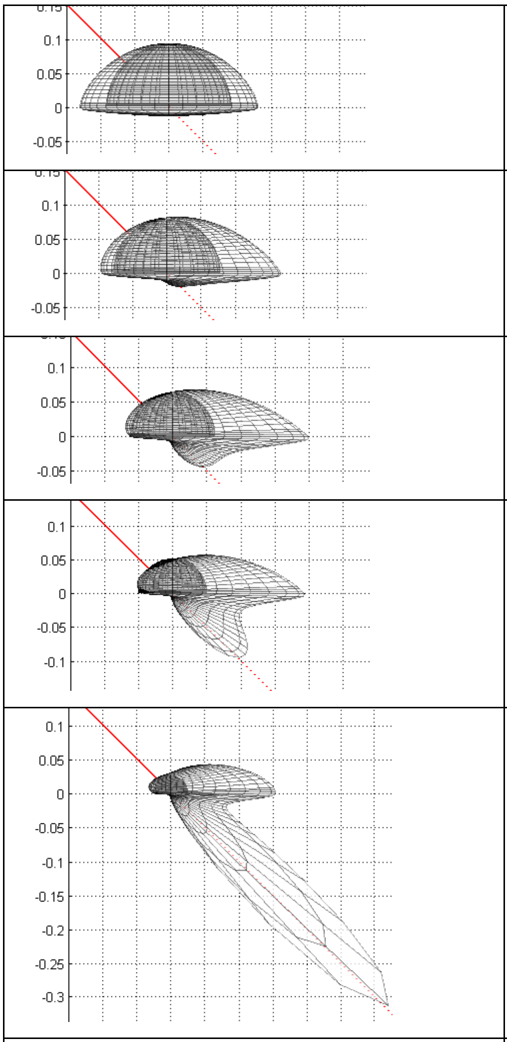

Figure 4a. Anisotropic light intensity in sample measured in ***45°/0°*** *instrument geometry for different asymmetry factors (from top: 0, 0.25, 0.50, 0.65, 0.80). Note that the device measures in the normal direction, and therefore incorrectly assumes the grey half sphere. Incident beam indicated as red line.*

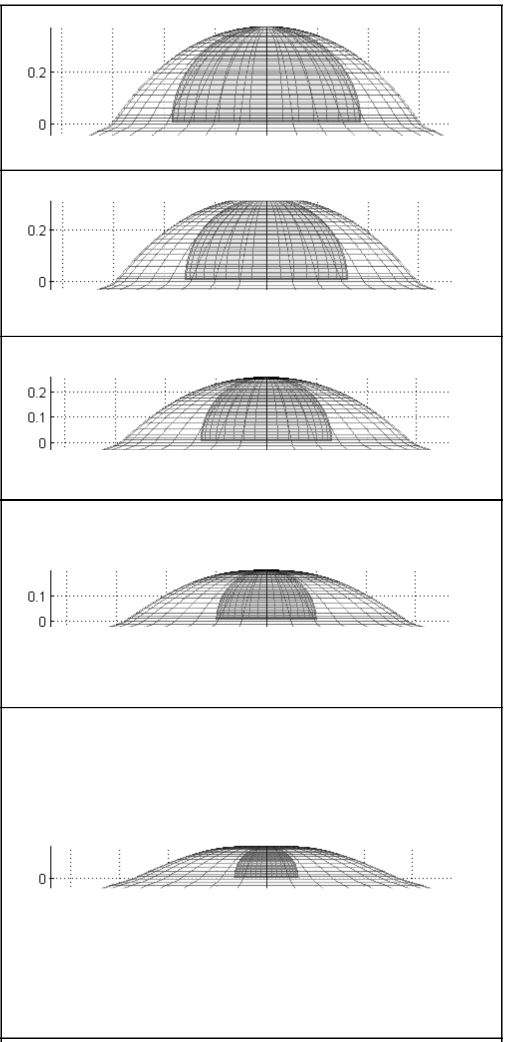

Figure 4b. Anisotropic light intensity in sample measured in ***d/0°*** *instrument geometry for different asymmetry factors (from top: 0, 0.25, 0.50, 0.65, 0.80). Note that the device measures in the normal direction, and therefore incorrectly assumes the grey half sphere.*

3.2. Eliminating Parameter Dependencies

It is clear from the last section that errors will arise when interpreting reflectance measurements with the Kubelka-Munk model. However, the most common ways to use Kubelka-Munk in practice reduces the effect of the errors [8], which is why the model is so useful. However, there are a number of cases where this is not the case, and where anomalous effects are reported.

One such case is the apparent dependencies between the Kubelka-Munk scattering and absorption coefficients for dyed paper samples [10-14]. Light scattering is largely due to the structure of the sample, which is not affected by the addition of dye. Therefore, identical paper samples with increasing amount of dye should have nearly similar scattering coefficients. However, it is reported how the scattering coefficient decreases in the region of absorption, and this has been interpreted as an intrinsic error of the Kubelka-Munk model. The top row of figure 5 illustrates this for dyed paper samples without and with fillers.

But, as can be seen already in figure 4, the errors arise from an over-idealized view of the instrument due to the fact that instrument readings are incorrectly interpreted. These errors can be larger than any errors inherent in the Kubelka-Munk model itself, even in idealized situations. In fact, the measurement device and the simulation model cannot be viewed as separate instances, which is a widespread implicit practice in applied reflectance measurements. Rather, given a measurement device, measurement data should be interpreted through a model that takes into consideration the actual geometry, function and calibration of the instrument. In the middle row of figure 5, the same measurement data are interpreted with the angle resolved model DORT2002 [8-9, 26] with a constant asymmetry factor, and the parameter dependencies are clearly reduced.

It can also be seen from figure 4 that another source of error is the failure to recognize the influence of a non-isotropic single scattering process. When making also spectral estimations of the asymmetry factor, which is what Kubelka-Munk already does for scattering and absorption, things should improve further. This requires goniophotometer measurements, which were here simulated for the same samples. The bottom row of figure 5 shows this case, where the parameter dependencies are now eliminated.

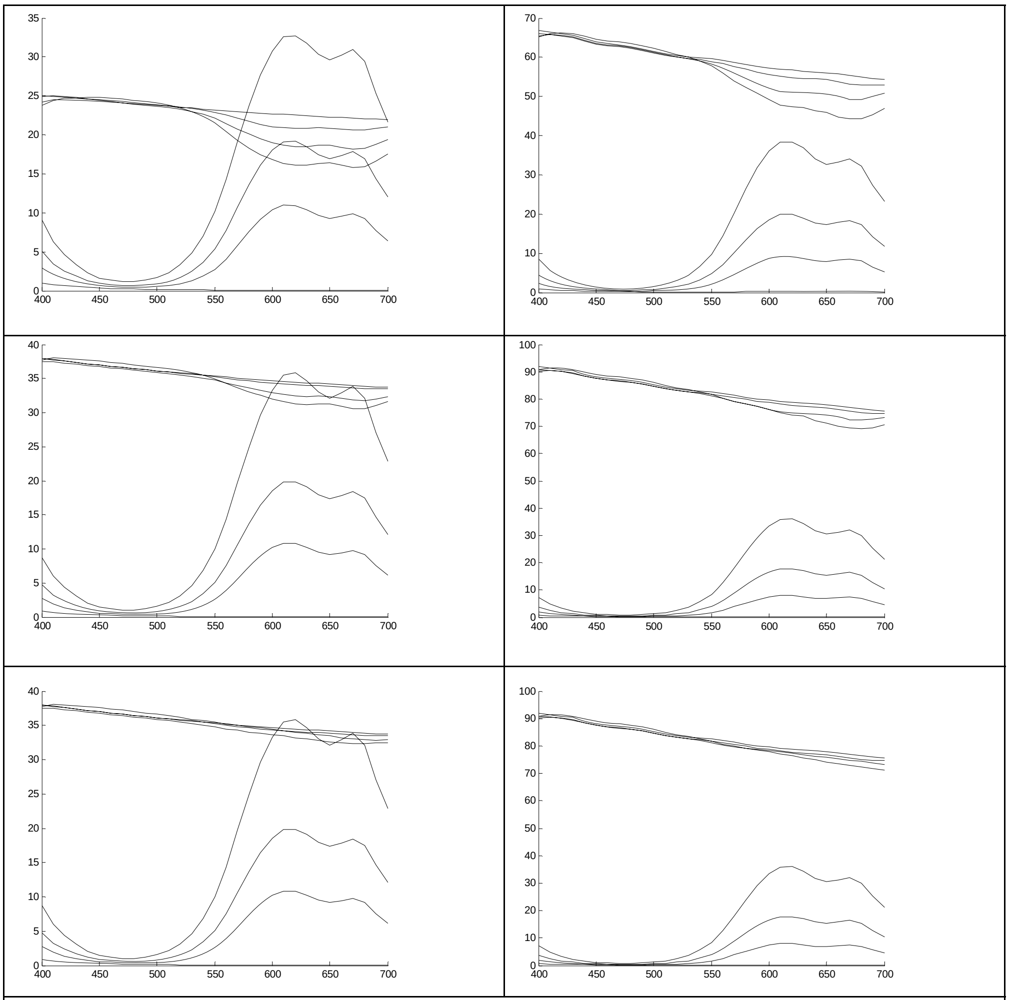

Figure 5.

Top: anomalous parameter dependencies for dyed samples, when measured according to ISO2469 [4] and calculated according to ISO9416 [7] (using Kubelka-Munk).

Middle: reduced parameter dependencies for dyed samples, when measured according to ISO2469 [4] and calculated with an angle resolved model (DORT2002, with asymmetry factor set to 0.8).

Bottom: eliminated parameter dependencies for dyed samples, when measured (here simulated) with a goniophotometer (to give spectral asymmetry factor values) and calculated with an angle resolved model (DORT2002).

Samples in the left column contain no fillers while samples in the right column contain fillers.

It is to be expected that further use of objective material parameters and models that can include the actual non-idealized measurement setup will resolve several outstanding issues related to anisotropy. One example is the possibility to get identical parameter values from measurements in different devices, such as mentioned in section 2.3.1. The radiative transfer based light scattering simulation tool DORT2002 offers these possibilities. It is in all aspects the Next Generation Kubelka-Munk, and provides a greater range of applicability, higher accuracy and increased understanding. It offers better interpretation of measurement data, and facilitates the exchange of data between the paper and graphical arts industries. It opens for understanding of anisotropic reflectance and for the utilization of the asymmetry factor to design anisotropy, and thereby for the design of different visual appearance or optical performance in new printed or paper products.

3.3. Other Effects of Anisotropy

Since optical anisotropy has not been treated much in the paper industry, not much is known of numerical values of the asymmetry factor for different paper constituents. Also, little is known of the effects of anisotropy.

As a couple of examples, the opacity and the reflectance factor over black background were calculated for identical samples with varying asymmetry factor. The simulations mimic the standardized d/0° measurement situation, and are illustrated in figure 6. It is clear how these quantities are markedly affected by the asymmetry factor. For the reflectance factor, it can also be seen that the 45°/0° and d/0° devices are differently affected, and that the ranking of samples actually shifts.

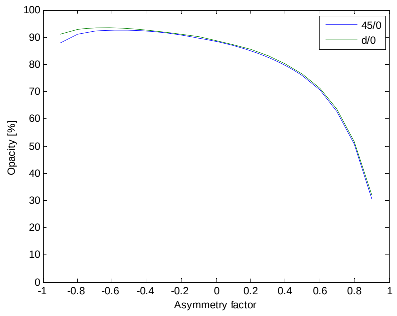

*Figure 6a. Opacity of sample as measured in **45°/0°** and **d/0°** instrument geometries for different asymmetry factors. Note the decrease in opacity for large asymmetry factors (0.3-0.8 are usual values for organic substances).*

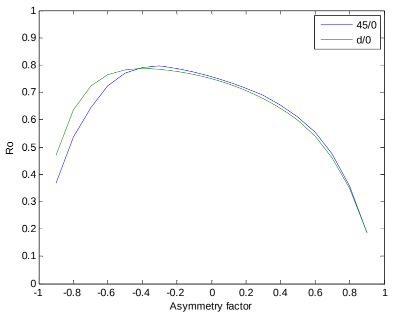

*Figure 6b. Reflectance factor over black background of sample as measured in **45°/0°** and **d/0°** instrument geometries for different asymmetry factors. Note the shift in rank for different asymmetry factors.*

Increased knowledge of anisotropy makes it possible to understand and control the phenomenon. It is to be expected that the Kubelka-Munk pair of scattering and absorption coefficients will be replaced by a triplet of physically objective scattering, absorption and asymmetry parameters, and that this will open a new area of material property design.

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