THREE-DIMENSIONAL MODELLING OF PAPER STRUCTURE: OPTICAL PROPERTIES OF PAPER AND PRINT

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Abstract: Three-dimensional models are developed for the structure of paper and for the detailed interaction of light with paper. The models are used in Monte Carlo simulations of the propagation of light in paper. The simulations are spatially and spectrally resolved and allow for features such as different structure in different layers of the paper as well as for ink printed on the paper. The models are used in numerical experiments in which individual structural parameters are changed and the effects on the optical properties of the paper studied. It is shown that both the detailed distribution of ink on and in the paper and the choice of model for the paper structure are important for modelling of print through and optical dot gain.

Introduction

When studying the influence of structure on the properties of paper, the structure must somehow be simplified and approximated. Often, when modelling the optical properties of paper, simplification is taken to the level of no structure remaining. The most well-known example of this is the Kubelka-Munk model (Kubelka *et al.*, 1931, Steele 1935, Kubelka, 1948, 1954). This model was originally devised to describe a layer of paint on a surface and it is based on the assumptions that the layer is homogeneous and isotropic, that it has a probability for absorption and a probability for scattering. It therefore leaves out effects related to a structure being made from fibres. Furthermore, it does not allow for the non-isotropic scattering against small particles, which in more simple cases is described as Rayleigh- or Mie-scattering.

Several models have been developed in which the layered structure of paper is included (Scallan *et al.*, 1972, 1974, Borsch, *et al.*, 1976, Scallan, 1985, Leskelä, 1993, 1994, 1995, Carlsson, *et al.*, 1995a). These models make a more or less one-dimensional description of the structure of paper, describing it as alternating layers of air and cellulose. In some cases fillers are also included.

The model of Carlsson *et al.* (1995b) makes a direct description of the three-dimensional fibre- and pore structure of paper. It describes the alignment of fibres in the plane of the paper, reflection of the light at fibre-pore interfaces and scattering against fine particles or small pores.

With print the three-dimensional complexity of the paper is further increased. This is because the distribution of ink both on and inside the sheet may have to be considered. With screen dots there is a two-dimensional distribution of ink over the surface. The ink may also penetrate significantly into the paper. The distribution of ink in the paper, or on its surface, interacts with the propagation of light inside the paper. In some cases not only the pigments of the ink have to be considered but also the ink vehicle, which affects the light scattering in the paper and which often has a spatial distribution different from that of the pigment.

Three-dimensional modelling

There are several reasons why modelling of paper, print and light may need to be three-dimensional: the paper structure, the distribution of light in the paper, the light scattering process and the distribution of ink in the paper. Three-dimensional modelling can mean quite different things, depending on which of these features are treated three-dimensionally. In order to model optical dot gain, for example, one has to introduce a two- or three-dimensional distribution of ink in the dot and study the three-dimensional distribution of light around it. But this can be done using a homogeneous model of the paper structure and an isotropic model for light scattering, giving a paper model equivalent to the Kubelka-Munk model, or it can be done with a three dimensional model of the fibre structure and with anisotropic light scattering.

In paper, with the majority of fibres aligned in the plane of the sheet, a non-isotropic layered structure is obtained. This gives the paper markedly different properties in the z-direction as compared with the machine- or cross directions. Due to fibre orientation machine-made paper also has somewhat different properties in the machine- and cross directions (see for example Schaffnit *et al.*, 1992). Paper has a three-dimensional fibre- and pore structure. One advantage of a model which describes this directly is the better and more direct understanding which is possible if one, as an example, can say that a change in opacity is due to a certain change in the pore size distribution rather than just saying that it is a change in the scattering coefficient.

Another type of paper structure is that which appears in coated paper and in paper with layers made from different pulps. These usually have to be described by different parameters or by completely different structure models.

Formation, the variation in local basis weight, is a two-dimensional variation in the plane of the paper. In order to model a real sheet structure formation should be included. That means that the parameters describing the structure should have a variation in the plane of the paper.

Paper structure

In the three-dimensional model (Carlsson *et al.*, 1995b) paper is made up of fibres and fine particles such as fillers or fines. Between the fibres there are pores.

The fibres are originally cylindrical but have been flattened and have, in this model, an elliptical cross section. The lumen is assumed to be collapsed. The fibres are placed horizontally in the paper sheet with the distribution of their longitudinal directions forming an ellipse. All fibres are straight and have the shape of a cylinder with an elliptical cross section.

Pores are the air filled spaces between fibres. At a fibre-pore interface light is reflected or transmitted. The probability for either is given by the Fresnel formulae, and depends on the refractive indices and the angle of incidence. If light is transmitted the refraction is given by Snell's law.

Fine particles or small pores causing the scattering of light are assumed to be situated on the surface of the fibres. At each fibre surface there is a probability for scattering. The angular distribution of the scattered light is determined by a phase function and an anisotropy parameter. The phase function which is used (1) was first introduced to describe light scattering in astrophysics (Henyey *et al.* 1941). In the equation θ is the scattering angle and g the anisotropy of the scattering, the expectation value of $\cos\theta$.

$$P(\cos\theta) = \frac{1-g^2}{2(1+g^2-2g\cos\theta)^{3/2}} \qquad (1)$$

This means that the complex angular distribution of the scattering against pores and particles of different size and shape is reduced to a fairly simple analytical expression. The anisotropy can be varied between -1 and 1. A value close to -1 means that scattering is strongly enhanced in the backward direction and a value close to 1 means that scattering is strongly enhanced in the forward direction. A value of 0 gives, with this distribution, isotropic scattering. An important result from Mie scattering is that scattering in the forward direction is much favoured.

The size of fibres and pores have distributions which can be chosen as part of the model. Other parameters of this model are the refractive indices of fibre and pore, the absorption cross section, the part of the fibre surface which is in direct contact with other fibres and the anisotropy of the fibre direction.

The three-dimensional model includes both scattering and reflection. Reflection is what may occur when light impinges on a surface, such as a mirror or a large enough cellulose fibre. This process follows simple geometrical laws. Scattering is what may occur if the surface is replaced by a particle, such as a filler particle or a small pore. There is no absolute limit between what is a particle and what is a surface but a particle should be comparable in size with the wavelength of the light, or smaller, and a surface should be considerably larger than the wavelength of the light.

The layered model (Carlsson *et al.*, 1995a) is a simplification of the three-dimensional model, with fibre structure considered only in the z-direction. In this model paper is described as alternating layers with different refractive index, *e.g.* cellulose and air. The thickness of the layers follow distributions which can be chosen as parts of the model. At the fibre-pore interfaces light is reflected or transmitted according to the Fresnel formulae and Snell's law. The scattering follows the phase function and anisotropy which were described above. Absorption is determined by an absorption cross section. In the case of no scattering the layered model becomes what is called the Stokes model. The Stokes model (Stokes, 1862) originally addresses a more fundamental optical problem: the reflectance of a set of parallel glass plates. The solution to this problem has later been found useful as a model for describing paper (Scallan *et al.*, 1972, 1974, Borsch, *et al.*, 1976, Scallan, 1985, Olf, 1988, 1989a, 1989b).

A furthermore simplified model is the homogeneous model. This assumes that the material is homogeneous with scattering and absorption. The absorption is described by an absorption cross section, the scattering by a scattering cross section, a phase function and an anisotropy parameter. In the case of isotropic scattering, $g=0$, the homogeneous model becomes equivalent to the Kubelka-Munk model.

These models can also be used for paper with print. The difference between printed and not printed paper is that the absorption is different, so by having different absorption cross section in different parts of the paper, print can be included in three-dimensional modelling. Often also the reflection- and scattering properties are different. With oil in the pores either their refractive index, or, if that is not included explicitly, the scattering cross section should be different.

Monte Carlo simulation of light propagation in paper

In the Monte Carlo simulations which are performed using the models discussed above, the light entering onto the sheet of paper is characterised by its wavelength, the number of photons, the direction of incidence of the individual photons and their spatial distribution.

Before a Monte Carlo simulation starts each of the parameters defining the paper structure, the light and their interaction is assigned a distribution or a value. The number of photons needed for a simulation depends on the statistical significance aimed at and on how complicated the studied situation is. More photons are for example needed to determine the angular distribution of the reflected light than just to determine the reflectance. Typically, the number of photons in a simulation is in the range 10^4 to 10^7. The time required for such a calculation ranges from a few seconds to a few hours, mainly depending on the number of photons but also on for example which model is used and how strong the absorption is.

In a simulation the photons are one by one sent on a random journey into the paper structure. Inside the sheet the photons encounter, depending on the model, fibres, pores and fine particles or simply a probability for scattering. Absorption also takes place along the path. When a photon encounters a fibre or a pore, parameter values describing the size and orientation of this are randomly chosen within their distributions. At each surface the probability for reflection and transmission is calculated. There is also a probability for scattering at each surface and when a photon is scattered this is in some random angle which depends on the anisotropy. There is also a probability for absorption related to how long path the photon travels inside the paper. During the passage of each photon through the structure the co-ordinates of the photon, its travelled distance and events such as scattering and absorption are monitored. Each photon is monitored until it either leaves the paper, as a reflected or transmitted photon, or until it is absorbed.

By collecting the statistics for a large number of photons, the optical properties of the paper, like reflectance and transmittance, are determined. For the reflected and transmitted photons the distance and time spent inside the paper, the point and at which angle they leave the paper are recorded.

By changing stepwise in a systematic way one or more of the parameters this type of simulation can be used to perform numerical experiments. The effects on the optical properties of a paper due to changes in structure or composition of the paper can be studied.

Often, optical measurements on paper are performed using diffuse light. One reason for this is that the Kubelka-Munk model assumes the light to be diffuse. Limiting the modelling to diffuse light reduces the types of measurements with which it can be used for evaluating the model. If the simulation model is made also to account for other light geometries it can be more generally evaluated by experiments. For example, angularly resolved measurements can give information both of the surface properties and of the bulk properties of the diffusely reflecting paper. An advantage of Monte Carlo simulations is that they can be performed for light with any particular property and are therefore compatible with any type of optical experiment.

Modelling of the optical properties of paper

The purpose of this modelling work is to study and describe the influence of structure on the optical properties of paper (Carlsson *et al.*, 1995b). An example showing the possibility to study changes in optical properties of a paper sheet under a process similar to calandering is illustrated in Figure 1. It shows the reflectance and transmittance for collimated light at 550 nm, calculated for sheets of paper with properties similar to those of newsprint. The fibre- and pore size distributions are the same in the different simulations, only the part of the total fibre surface which is in direct contact with other fibres is changed. The basis weight is fixed at 65 g/m^2. This means that all sheets have the same fibres, but the density of the sheets varies. With less fibre-fibre contact, there are more pores and more surface is free to contribute to the scattering or reflection of light. This makes the sheet less transparent. With more pores the density becomes lower. Table 1 gives the densities which can be calculated for these structures, assuming a fibre density of 1000 kg/m^3. A density of around 650 kg/m^3, as for newsprint, gives a free fibre ratio between 0.5 and 0.6 in this model and optical properties agreeing with what would be expected for such paper.

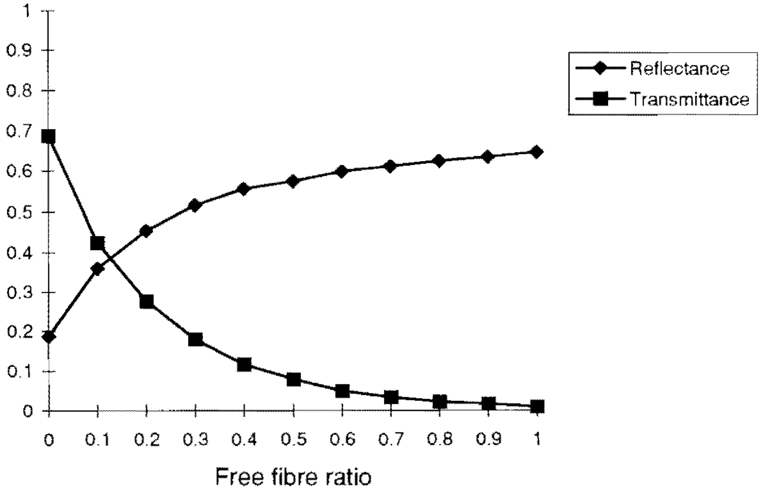

Figure 1. Calculated reflectance and transmittance values as functions of the part of the fibre surface not in contact with other fibres. All sheets have the same basis weight.

Free fibre ratio	Density (kg/m^3)
0.0	1000
0.1	912
0.2	838
0.3	775
0.4	722
0.5	675
0.6	633
0.7	596
0.8	564
0.9	538
1.0	509

Table 1. Densities calculated for the structures used for Figure 1.

Print through is caused by the penetration of the ink pigment and, particularly for oil-based ink, the penetration of the ink vehicle into the paper and by the diffuse reflectance of light whereby it is scattered inside the paper. This problem involves the z-direction variation of the absorption and scattering caused by the ink and the three-dimensional distribution of light inside the paper.

The calculations for paper with print are compared with reflection- and transmission measurements. These measurements are made using a high-pressure xenon lamp and an integrating sphere equipped with a spectrometer and a CCD detector. By recording the spectrum of light that is transmitted by one sheet and dividing this with a similar recording of the light from the lamp, an absolute transmittance spectrum is obtained. In the same way, for the light that is reflected by one sheet an absolute reflectance spectrum is obtained and for the light that is reflected by a pile of sheets, a reflectivity spectrum. This is illustrated in Figure 2 which shows the results for a newsprint. Such measurements are also made for paper with print on either the front- or back side. From these measurements information on print through and dot gain can be obtained.

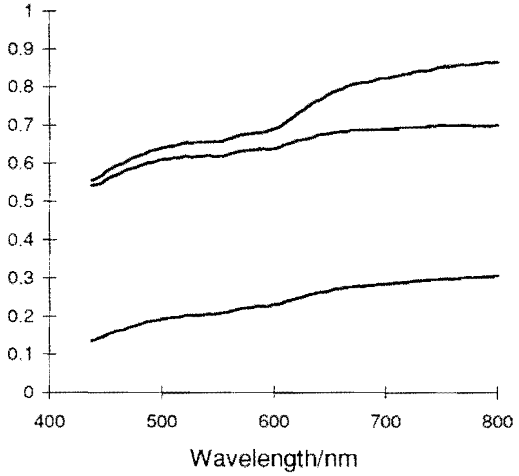

Figure 2. Reflectivity, reflectance and transmittance (top to bottom) of a newsprint, measured as functions of the wavelength.

Figure 3 shows the wavelength dependence of print through for different colours on newsprint. In the figure the ratio is given of the reflectivity measured for a pile of sheets with print on the back of the first one and the reflectivity of the same pile without the printed sheet. The print through is strongly wavelength dependent. The reasons for this are the varying absorption of the ink and the different propagation of light at different wavelengths. The effect of the latter is best seen for the black print.

In order to model these results, the optical properties of not printed paper (reflectivity, reflectance and transmittance) were used for determining the parameters of the three-dimensional model. All parameters except the absorption cross section were fixed to be the same at all wavelengths. Figure 4 shows the results obtained when black print was added to this model, either on the surface or with a penetration depth of 15 μm into the 70 μm thick sheet. With print only on the surface print through is underestimated while a penetration of 15 μm gives results in reasonable agreement with experiment. This penetration depth is consistent with previous measurements of ink penetration in newsprint (Larsson *et al.*, 1972).

With the spectral resolution of these models not only the change of intensity with print on the back of a paper is calculated. Also the effect on the colour is obtained. For example, the black print of Figure 4, which absorbs mainly in the red region of the spectrum, appears blue-green when compared with the paper without print. The cause of this is the absorption of the lignin. This absorption is strongest at short wavelengths, transmitting the longer wavelengths to be absorbed by the print on the back.

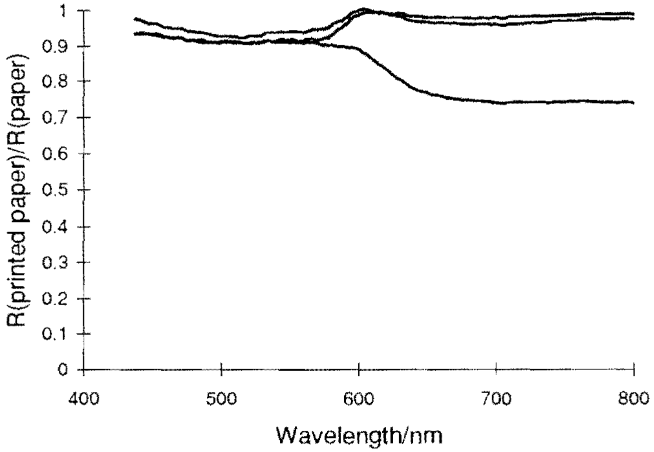

Figure 3. Measured print through for (top to bottom) magenta, red and black print on newsprint.

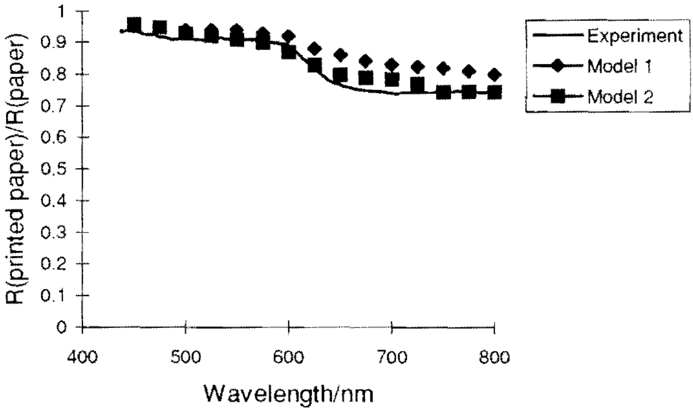

Figure 4. Calculated print through with ink on the surface only (Model 1) or with 15 μm penetration (Model 2).

Optical dot gain is often described by the Yule-Nielsen equation (Yule *et al.*, 1951), which says that with a given area fraction of the dots, F, the reflectivity of a halftone print, R(F), can be calculated from the reflectivity of the unprinted paper, R_{paper}, and the reflectivity of a full tone print, R_{print}, according to

$$R(F) = \left[F R_{print}^{1/n} + (1-F) R_{paper}^{1/n} \right]^{n} \qquad (2)$$

If n=1 this gives the Murray-Davies equation (Murray, 1936) which corresponds to no optical dot gain. For most papers the value of n is between 1 and 2. The parameter n has no direct physical meaning but depends on the dot geometry and on the structure of the paper. Other models have been suggested, using other empirical parameters (Arney *et al.*, 1995, 1996a, 1996b). One advantage of describing optical dot gain in three-dimensional modelling (Kruse *et al.*, 1995, Carlsson *et al.*, 1995b, Wedin 1995, Gustavson, 1995) is that the description is made directly in the parameters describing the paper structure and the dot geometry. Light scattering at print edges has been described with a method consistent with the Kubelka-Munk model (Engeldrum *et al.*, 1995).

Above, dot gain was discussed in terms of print density. This is a somewhat indirect measure. It describes what happens with the printed surface whereas the origin of optical dot gain is a local effect in or around each dot. Lately, dot gain has been studied also at this local level by comparing the physical size of the printed dots with that of the optical image of the same dots (Nilsson *et al.*, 1997).

Screen dots printed on a sheet of paper require, in the general case, a three-dimensional description of the ink distribution. The influence of ink penetration into the paper is illustrated in Figure 5. It shows the calculated reflected intensity around a black circular dot on paper. The homogeneous model has been used with isotropic scattering. The only difference between the two simulations is that in one of them the ink is on the surface of the paper, in the other one it has penetrated 20 μm into it, with a homogeneous distribution down to that depth. The penetration of ink into the paper does in this case give a larger optical dot gain.

Figure 5 illustrates the importance of including the z-dependence of the ink distribution while the distribution in the plane of the paper was assumed to be circular and homogeneous. In many cases the distribution is much more irregular, this can be seen for example in Nilsson *et al.* (1997). The uneven distribution of ink makes the borderline of the dot much longer than it would have been for a circular dot. This is particularly important since optical dot gain is an effect which happens at the border between the printed and not printed paper.

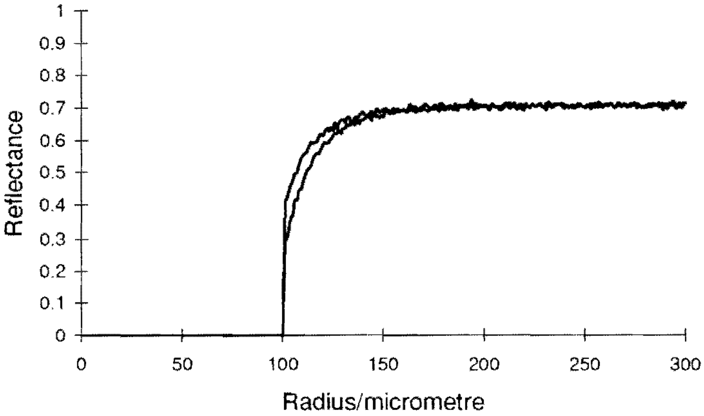

Figure 5. Reflected intensity around a black screen dot with 100 μm physical radius. The intensity along a radius from the centre of the dot is shown. The two curves show the results for a dot on the surface (smaller dot gain) and with 20 μm penetration into the paper (larger dot gain) on the same paper model.

The paper structure influences how light propagates inside the paper and therefore also the optical dot gain. The importance of the model used for the paper structure is illustrated in Figure 6. It shows the light reflected around a 100 μm black screen dot on the surface of a paper sheet modelled according to three different paper structure models: the homogeneous model with isotropic scattering, the layered model and the three-dimensional model. The parameters have been chosen so that all models give the same reflectance and transmittance. The paper models look the same in reflection and transmission but the dot gain differs significantly. Without comparing with experiments one can not say which one is more correct. What one can say, however, is that the way that fibre structure is described influences the calculated optical dot gain and that the influence of the structure should therefore be considered in the modelling.

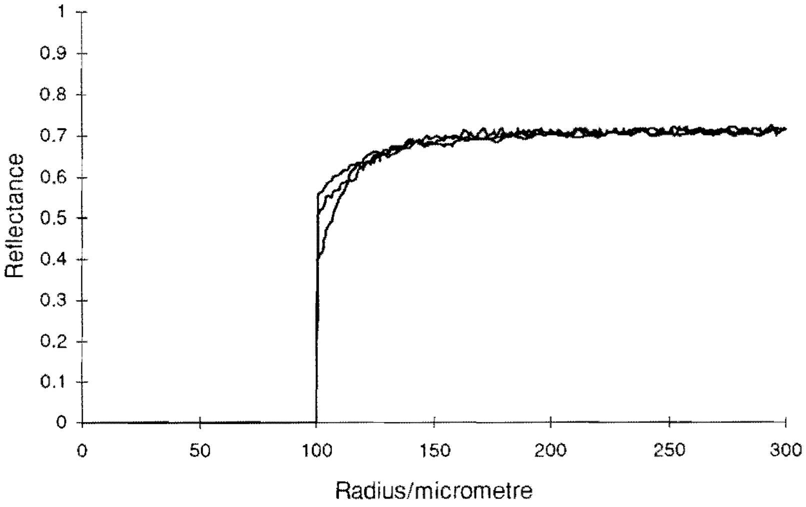

Figure 6. Reflected intensity around a black screen dot with 100 μm physical radius. The intensity along a radius from the centre of the dot is shown. The three curves show the results for a dot on the surface using the homogeneous model (largest dot gain), the layered model (smallest dot gain) and the three-dimensional model. All models give the same reflectance and transmittance.

Conclusions

When modelling the interaction of light with printed paper both the detailed distribution of ink on and in the paper and the way that the model describes the paper structure are important. Using Monte-Carlo simulations three-dimensional modelling can be performed for the fibre structure of the paper, the distribution of ink in the paper as well as for the propagation of light in the printed paper.

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