Some Ideas on Models and Methods for Light Scattering in Paper

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Some Ideas on Models and Methods for Light Scattering in Paper

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Abstract

In this report a short overview is given on existing models for simulating light scattering in paper. The well known Kubelka-Munk model somewhat oversimplifies the problem. Newer discrete ordinate models take into account more aspects, e.g. angle resolved scattering, but have intrinsic ill-conditioned problems that have to be overcome. No existing models are designed to solve the inverse problem, i.e. finding model parameters given real light scattering measurements.

Therefore we propose a Stable Multilayer Discrete Ordinate Radiative Transfer model, SM-DORT, to simulate the scattering of light in coated paper and similar structures, and to solve the corresponding inverse problem. We discuss improvements of existing models, for making SM-DORT stable to give reliable results in spite of intrinsic ill-conditioned problems, and for making it fast to efficiently solve the inverse problem.

In this report we also cover some aspects of inverse problems in general, we give some ideas on further model improvement to take into account more aspects of light scattering in paper, and we discuss model validation, using experiments and existing models.

Keywords: Light scattering, radiative transfer, inverse problems.
Introduction

The modelling of light scattering in paper is an interesting application of light scattering with difficulties that are not easily resolved. This report will give a short description of light scattering in paper with the emphasis on computational aspects for evaluating different existing models. We also suggest how to improve and extend the existent implementation of the DORT model.

A model can be trusted only if it is evaluated against some kind of measurements. This evaluation can be performed experimentally using a clever set of experiments in order to find unknown parameters or just confirming the validity of the model. However, it is generally of more value if a model is actually optimised against the given measurements. When fitting models to given data an optimisation problem has to be solved. These kinds of optimisation problems have certain properties that we intend to describe briefly. We believe that this is a non-trivial part of the building and evaluation of models and an important aspect of the modelling of light scattering in paper.

Models

Discrete Ordinate Models

Radiative transfer has been covered in numerous articles, from different approaches. The general problem has no analytical solution, but a suitable coordinate system will simplify it. A commonly used coordinate system in radiative transfer is a spherical one (r, φ, θ). If we are only interested in the angular distribution of the radiation, the r-coordinate becomes irrelevant. Assuming azimuthal symmetry allows us to drop the φ-coordinate as well. If this is not possible, there are ways to separate the φ-dependence, e.g. expanding in a Fourier series, and thus solving several φ-independent problems. This leaves us with the single θ-coordinate.

To further simplify the problem, it is usual to make a discrete approximation for the θ-coordinate. This divides the space into cones, commonly referred to as channels, see figure to the right. In the old Cartesian coordinate system, the vertical coordinate was called ordinate (as opposed to abscissa), and so these models are known as discrete ordinate models. Sometimes they are also referred to as many-flux models.

The first to use such a coordinate system for radiative transfer calculations was Schuster¹, who used only two channels, one for light propagating in a forward direction, and one for backward direction. Many authors have adopted this approach, the most known of which are Kubelka and Munk.
Pursuing his interest in the scattering of neutrons, Wick\textsuperscript{2} was the first to generalize this approach to several channels. Later, Chandrasekhar\textsuperscript{3} applied this method to radiative transfer, examining it thoroughly.

Discrete ordinate methods were for a long time considered to be practically useless, because they give rise to eigenvalue problems for large, unsymmetrical matrices. Not until sophisticated algorithms for the eigenvalue problem became available, the methods were more exploited. Below we discuss the Kubelka-Munk model, two different kinds of discrete ordinate methods, and suggest a new improved model.

### The Kubelka-Munk model

Perhaps the first model of light scattering in paper was developed by Kubelka and Munk\textsuperscript{4} in the 1930s. The model is based on the assumption that both the incident and scattered light is totally diffuse. Therefore, much of the standard measurements are made under the assumption of diffuse light. The main assumptions for the Kubelka-Munk theory are the following.

- The medium has a continuous and homogeneous distribution of scattering sites.
- The medium is infinite in the plane of the paper but has a finite thickness.
- The angular distribution is perfectly diffuse (so called Lambertian).
- No light is emitted in the medium.

In order to give some details we define $R$ as the reflectance at the surface, i.e., the quotient $I/J$ where $I$ is the incident intensity and $J$ is the reflected intensity of light. $R_\infty$ is the reflectance of the paper for a very thick pile of paper. By doing an analysis with a layer of infinitely small thickness it is possible to derive closed expressions for the reflectance $s$ and absorption $k$ as a function of $R$, $R_\infty$, and the thickness or grammage (also referred to as the normalising parameter). An important relation in the theory is the equation

$$1 + \frac{k}{s} = \sqrt{\left(\frac{k}{s}\right)^2 + 2\left(\frac{k}{s}\right)} = R_\infty$$

that relates a measurable quantity to the quotient $k/s$ directly. The obvious advantage of the Kubelka-Munk theory is that the measured quantities (reflectance factors) are directly related to the parameters of the model ($s$ and $k$). This means that we do not have to solve any inverse problem at all in order to attain the parameters of the model. However, the model is quite crude and the computational savings is not an argument for not considering more sophisticated models.

For a more thorough description of the Kubelka-Munk theory we refer to the report of Hjalmar Granberg\textsuperscript{5}. 

The DORT model

The Kubelka-Munk model somewhat oversimplifies the problem by considering radiation in only two directions – upwards and downwards. Although a simple model, it has been commonly used since it is fast and easy to use. However, this model cannot provide information about the angular distribution of the transmitted and scattered light, nor does it include any surface contributions to scattering.

To include angular distribution, Mudgett and Richards, starting with Schuster’s ideas, outlined a discrete ordinate model with several channels. Their main interest was in the optics of paint films. Later, Berglind proposed a straightforward implementation of this model, which hereafter will be referred to as DORT.

For the ease of comparison with the next discrete ordinate model, the main characteristics of DORT are listed here.

1. The scattering medium is assumed to be isotropic and homogeneous.
2. The formulas are restricted to a scattering medium bounded by parallel planes, extending over a large region compared to its thickness.
3. Incoming radiation is assumed unpolarized, but may be diffuse or directed, or a mixture of both.
4. Emission or fluorescence within the scattering medium is not included.
5. The model is monochromatic, or the radiation is confined to a narrow enough wavelength range that the model parameters are constant.
6. DORT will give the flux anywhere, inside or outside the media.
7. DORT does not explicitly use the thickness of the media in the solution procedure.
8. DORT assumes all parameters to be constant within each medium.
9. DORT assumes azimuthal symmetry.
10. DORT is developed for handling several layers – with different parameters, including different index of refraction – in optical contact. Snell’s law and the Fresnel formulas are applied at the layer boundaries. Solving the problem for one layer, including boundaries, yields a general reflection matrix and a general transmission matrix, describing the amount of flux being reflected and transmitted from one channel to another after the light has passed through the layer. These matrices are then used when solving for the next layer. This process can be repeated for an arbitrary number of layers, thus giving a multilayer solution.
11. The MATLAB code of Berglind’s straightforward implementation of DORT is not publicly available. Unfortunately it suffers from numerical difficulties, and it is not obvious that the results are reliable. The numerical problems arise in solving the eigenvalue problem, and in the system of equations used for solving for the constants of integration. These problems are often ill conditioned, and MATLAB’s built-in standard routines do not always give reliable results.
12. DORT has recently been adopted by the paper industry to be used in optical design, due to its ability to simulate angle-resolved scattering, and the scattering of light in
multilayered structures with different index of refraction in different layers, such as coated paper.
The DISORT model

Stamnes\(^8\), using ideas from Wick and Chandrasekhar, presented a thorough examination of the theory and numerical implementations of the problem, and proposed a model for light scattering in the atmosphere. This model will hereafter be referred to as DISORT.

For the ease of comparison with DORT, the main characteristics of DISORT are listed here, in the same order as for DORT.

1. The scattering medium is assumed to be isotropic and horizontally homogeneous, but may be vertically inhomogeneous.
2. The formulas are restricted to a scattering medium bounded by parallel planes. The medium may be very thick.
3. Incoming radiation is assumed unpolarized, but may be diffuse or directed, or a mixture of both.
4. Emission or fluorescence within the scattering medium is included.
5. The model is monochromatic, or the radiation is confined to a narrow enough wavelength range that the model parameters are constant.
6. DISORT will give the flux only inside the medium.
7. DISORT does explicitly use the thickness of the media in the solution procedure, by assuming the medium to consist of a number of adjacent homogenous sub layers, solving for each homogenous sub layer, and integrating for the total solution.
8. DISORT allows the parameters to be continuously varying vertically inside the medium, by approximating the continuous variation by a step-function variation, corresponding to the homogenous sub layers. The index of refraction, though, is not allowed to vary.
9. DISORT does not assume azimuthal symmetry. Instead, the \( \varphi \)-dependence is separated, and by expanding in a Fourier series, the problem is transformed into solving several \( \varphi \)-independent problems. Finally a \( \varphi \)-dependent solution is put together. In fact, one might say that DISORT solves a generalized single-layer DORT-problem for each \( \varphi \)-component.
10. DISORT is developed for handling only one layer – although an extension for two layers (atmosphere/ocean) with different index of refraction has recently been developed\(^9\).
11. The FORTRAN code of DISORT has been made publicly available, together with a thorough examination of the theory and the numerical implementation. What Stamnes calls “the heart of DISORT” is a customized eigenvalue problem solver, which assumes that the eigenvalues are a priori known to be real (a consequence of the fact that the phase function depends only on scattering angle, and of having chosen a Gaussian quadrature rule). The customized routine is fast and stable. The ill-conditioned system of equations used for solving for the constants of integration is handled with a scaling transformation, which makes it unconditionally stable.
12. DISORT is well known and documented, and has thousands of users around the world, primarily in the field of atmospheric radiative transfer. It has also become a kind of standard against which to compare other modelling results. It was designed to be a software tool for others to use in various applications.
The GRACE model

To take into account the three-dimensional nature of the paper structure, a Monte Carlo simulation model, GRACE, was recently proposed by Hainzl\textsuperscript{10}. The main advantage of this model would be to contribute to the understanding of the physical processes of light scattering in paper.

The GRACE model can take into account any rule or parameter describing light interaction with any component in the paper structure. The model does not require any restrictions for the media, the radiation or the boundaries, and can therefore – when refined – be used to model real paper in a real environment.

At the same time the ability to model “the real world” is the greatest disadvantage of GRACE, since it involves substantially more parameters, many of which are unknown or difficult to measure. Furthermore, the calculation time increases tremendously, since the paper structure is modelled as a statistical distribution, and therefore hundreds of thousands or millions of wave packets need to interact with the paper structure in a simulation.

Inverse Problems

The problem class of inverse problems is large and complex. Generally an inverse problem exists only if we have a direct problem. The direct problem is the formulation of the evaluation of a model. As examples we can take differential equations like the heat equation or the Navier-Stokes equations but we can also have a more non-mathematical direct problem like the minimization of risk in a decision model. As an additional component in the inverse problem we assume that it contains some unknown quantity like, e.g., a boundary value, material parameters, or a function describing conductivity. The inverse problem is to find these unknown quantities given some additional information like measurements or control requirements.

The inverse problem is generally more difficult to solve than the direct problem since the direct problem has to be utilized in some sense during the actual solving of the inverse problem. Moreover, due to lack of information, the inverse problem is often ill posed in the sense that it has no solution or no unique solution. In order to attain any solution, the ill posed problem may be reformulated by adding more or less artificial information like the probable size of the solution or the exclusion of unwanted solutions. The reformulation of an ill posed problem is called regularization and is well known in some research areas such as control theory and image analysis but fairly unknown in other areas like design optimisation and VR technology.

The concepts in inverse problems described so far all applies to the optimisation or calibration of light scattering models. However, each model has its own mathematical characteristics making the direct problem more or less complex. Moreover, the inverse problem in light scattering is dependent on available information, i.e., experiments. The better we can use our
experiments the more certain it is that the inverse problem is well posed and has a physically relevant solution.

**Inverse scattering**

Inverse scattering\(^{11,12}\) is one example of an inverse problem where information about an unknown object is to be recovered from measurements of waves or fields scattered by this object. There seems to be very little work done in this area regarding light scattering in paper (as far as the authors are aware) so there is no possibility in this report to give any examples of inverse scattering in paper.

As a first example we consider the problem of determining a spatially varying acoustic profile \(n(x)\) which equals 1 outside some compact set. We assume that the harmonic incident wave is

\[
U^i(x,t) = e^{ikt}u^i(x)
\]

travelling with a speed 1. The scattered wave is

\[
U^s(x,t) = e^{ikt}u^s(x)
\]

and the total wave is then

\[
U(x,t) = e^{ikt}u(x) = e^{ikt}u^i(x) + e^{ikt}u^s(x)
\]

satisfying the wave equation

\[
U_{tt} - \frac{1}{n^2} \Delta U = 0,
\]

where \(1/n(x)\) is the speed in the medium. If we only consider the spatial part of the wave it is easily seen that from the wave equation we attain the so-called reduced wave equation or the Helmholtz equation

\[
\Delta u + k^2 n^2 u = 0.
\]

In the same manner it can be shown that the scattered wave satisfies

\[
\Delta u^s + k^2 n^2 u^s = k^2 (1-n^2)(u^i + u^s).
\]

The inverse scattering problem now consists in computing the unknown function \(n(x)\) from \(u(x)\) and \(u^i(x)\). Note that the determination of \(n(x)\) is a non-linear problem (due to the right hand side in the Poisson equation) even if the actual differential equation is linear. Further, any
measurements of \( u(x) \) and \( u'(x) \) are not possible because they can only be measured far from the support of \( n \), and the forming of the Laplacian from a noisy function will introduce too much errors. Thus, the inverse scattering problem is generally a non-linear ill posed problem.

The second example is the determination of the shape of a scatterer \( D \). The direct problem to be solved is the Helmholtz equation on the complement of \( D \) with some appropriate boundary conditions. In order to attain a unique solution of the direct problem, some additional assumption on the scattered field far from the solution is added. One example of such a condition is the Sommerfeld radiation condition

\[
\lim_{r \to \infty} \sqrt{r} (\frac{\partial u'}{\partial r} - iku') = 0, r = |x|
\]

that should be satisfied uniformly in all directions. Because of the Sommerfeld radiation condition the scattered wave has the asymptotic behaviour

\[
u'(x) = \lim_{r \to \infty} \frac{e^{i\theta}}{r} \left( u_w(\hat{x}) + O\left(\frac{1}{r}\right)\right), |x| \to \infty
\]

where \( \hat{x} = x/|x| \) and where the function \( u_w \) is called the far field pattern of the scattered wave. The fundamental inverse obstacle pattern scattering problem is now, given the far field pattern for one incident wave \( u'(x) = e^{ikx} \), to determine the shape of the scatterer \( D \). Much work has been done analysing this problem and there exist several algorithms for solving it.

**Solving Inverse Problems**

As mentioned above an inverse problem is difficult to solve because of its complexity and that it may be an ill posed problem. We will try to describe some methods that can deal with these two complications.

First, we may distinguish between inverse problems that include unknown functions and those that do not. If we begin with the latter case and consider only parameter estimation problems we may formulate such problems as some minimization problem

\[
\min_{\alpha} F(u(\alpha), \alpha)
\]

where \( \alpha \) is an unknown parameter vector, \( F \) is the function that measures the fit of the model, and \( u(\alpha) \) is the solution of the direct problem. Any minimization algorithm like the Gauss-Newton\(^{13}\) or Newton\(^{14}\) method can be applied to this problem. However, the more derivatives
that are needed by the minimization algorithm the more calculations are needed for finding the solution. Let us take some examples.

Consider the DORT model and assume that we have some measurements of the Reflectance factor that are to be fitted to the model. The minimization problem using a least squares formulation could look something like

\[ \min_{s, k, g} \sum \left| R_{i}^{\text{DORT}}(s, k, g) - R_{i}^{\text{MEAS}} \right|^2, \]

where \( R_{i}^{\text{DORT}} \) denotes the Reflectance factor given by the DORT model at scattering angle \( \theta_i \). In the DORT model it is quite possible to derive the derivatives of \( R_{i}^{\text{DORT}} \) with respect to \( s, k \) and \( g \) analytically that will give a very efficient evaluation of the derivatives (this is certainly not a trivial task). This will enable a DORT model to be fitted very efficiently to given data. Further, an efficient implementation makes it possible to handle space varying parameters and additional complexity in the model that includes additional free parameters and parameter functions. As an example we may take a non-linear density distribution of ink penetration\(^{15}\). At this date it is not known whether inverse problems using the DORT model are ill posed in, e.g., a space varying parameter.

If we consider the GRACE model and want to fit some of its parameters to some given data, it is in some sense more difficult. The reason is that we have no explicit mathematically formulated model in GRACE. The solution of the direct problem, i.e., the evaluation of the model is performed by a simulation. Any calculation of derivatives with respect to the parameters generally has to be performed by finite differences. Since one simulation alone takes hours the inverse problem using finite differences is, at this moment, intractable. However, interesting future research would be to investigate the possibilities of efficiently solving inverse problems where a Monte-Carlo method is used for the direct problem. The main idea for this research would be to use techniques like automatic differentiation that has been successfully applied, e.g., to artificial neural networks\(^{16}\).

If we assume that the problem is ill posed it is important that the algorithm for solving the minimization problem can handle this additional difficulty. There exist several different methods for handling ill posed problems that differs depending on the properties of the ill posedness. For further reading on this subject we refer to the work of Tarantola\(^{17}\) and Engl et al.\(^{18}\).

Future Model Development

Suggestion of a new stable model that handles several layers

Recently, the paper industry has shown an increased interest in radiative transfer theory, in order to simulate and predict light scattering in paper. The Kubelka-Munk model has been
used a long time, but the paper industry now needs a less simplified model. For example, one
wants to model gloss, asymmetry, diffuse scattering from rough surfaces, angle resolved
scattering, and distinguish between surface and bulk contributions to scattering. Further, it is of
interest to be able to solve for parameters such as asymmetry, scattering and absorption
coefficients, given angle resolved measurements.

Therefore we propose a Stable Multilayer Discrete Ordinate Radiative Transfer model, SM-
DORT, primarily to simulate the scattering of light in coated paper and similar structures. The
model needs to be stable to give reliable results, in spite of any intrinsic ill-conditioned
problems. SM-DORT needs to be fast to efficiently solve the inverse scattering problem, since
the parameter optimisation will require the model to be evaluated a large number of times.

Stability can be achieved by using ideas from DISORT for bulk scattering. The handling of
several layers with different index of refraction in different layers can be developed starting
from the ideas in DORT. However, SM-DORT will need to be written from scratch, only
using the ideas from DORT and DISORT, since the present implementations are far from
compatible.

Validation using existing models

Some simulations are suggested below to evaluate SM-DORT against other models. It would
be interesting to compare physical relevance, as well as computational speed. When
applicable, the simulations should be complemented with real measurements.

Since Kubelka-Munk is essentially a simple two-channel DORT model, it would be interesting
to simulate Kubelka-Munk and SM-DORT with two channels (and all other conditions
prescribed by Kubelka-Munk), and compare the results for total reflectance and total
transmittance, or scattering and absorption coefficients. If they agree, and if SM-DORT is
sufficiently fast, SM-DORT can completely replace Kubelka-Munk, since it has a wider range
of applicability, and gives information about angle distributed scattering, asymmetry and
surface contributions to scattering.

As mentioned above, DISORT is considered a standard against which to compare other
modelling results. Therefore, one should simulate DISORT and SM-DORT with one thin
homogeneous layer and the same number of channels, and compare the results for angle
resolved scattering, or scattering, absorption and asymmetry coefficients. If they agree, SM-
DORT can be considered to give correct results for bulk scattering according to radiative
transfer theory.

Furthermore, one should simulate DISORT and SM-DORT with internal sources or
fluorescence (and with one thin homogeneous layer and the same number of channels), and
compare the results. If they agree, SM-DORT can be considered to give correct results for
bulk scattering including internal sources or fluorescence.
Being designed for handling layers with different index of refraction, DORT could be used to evaluate different approaches of modelling surface scattering. Simulating DORT and SM-DORT with two or more thin homogeneous layers with different index of refraction and the same number of channels, could give information on this. For the same reason, DISORT with the extension for two layers and SM-DORT should be simulated with two thin homogeneous layers with different index of refraction and the same number of channels. If the results agree, SM-DORT can probably be considered to give correct results for surface scattering.

Since GRACE simulates “the real world”, it would be interesting to simulate GRACE and SM-DORT with different simple set-ups, and compare the results. This can be a way of comparing physical relevance for different parameters.

A way of evaluating different approaches of modelling diffuse scattering due to surface roughness could be to simulate GRACE and SM-DORT with one homogeneous layer and surface roughness, and compare the results.

Different approaches of modelling surface scattering, “effective index of refraction”, or partial optical contact, could be evaluated by simulating GRACE and SM-DORT with two or more thin homogeneous layers with different index of refraction.

**Further model improvement**

A new modelling approach should be considered for surface scattering in the cases when the media are not in perfect optical contact, or when different materials are mixed at the boundary. Berglind has suggested an “effective index of refraction” for a thin intermediary layer, which should be investigated further. Another way could be to introduce a parameter for partial or fractional optical contact, and consider a way of modifying the Fresnel formulas in accordance with that. It should also be investigated whether other sciences, such as chemistry, can contribute with knowledge on how different media interact at boundaries.

Emission or fluorescence within the scattering medium is included in DISORT. It should be investigated whether it can be included in SM-DORT to simulate fluorescence in paper.

The ability to model diffuse scattering from rough surfaces, and therefore gloss, needs a more thorough investigation. Berglind gave some suggestions, but more studies are needed on how to measure, characterize and model surface roughness.

An important question that should be answered is whether the scattering and absorption parameters really are independent. They are probably a function of the wavelength and this could be included in the model by solving an inverse problem in an appropriate function space.

**Robust algorithms**
Although having suggested that DISORT be used in SM-DORT for bulk scattering, it should be investigated whether a division in sub layers is necessary for the relatively thin layers considered here, since it would save a considerable amount of computations. For the same reason, it should be investigated whether a $\varphi$-dependent solution is needed, or if azimuthal symmetry can be assumed.

To save computations, some effort should be made to investigate how many channels are needed for the bulk scattering problem to achieve the desired angular resolution. As pointed out by Stamnes, the polar angles necessary for computational purposes are entirely decoupled from the polar angles at which results are given, and thus DISORT can use less channels than would otherwise be used.

The angular scattering pattern in bulk scattering is described with a phase function, which for computational reasons is expanded into a series of Legendre polynomials, which may be hundreds of terms long. Since all these polynomials of all degrees must be evaluated at all quadrature angles (channels) and output angles, this renders a large amount of calculations. Therefore, again, reducing the number of channels would save computations. But reducing the number of terms in the Legendre polynomials would save even more.

However, as first pointed out by Chandrasekhar, the number of channels must exceed the number of terms in the phase function expansion, which would yield several hundreds of channels and impossibly large computations. Thus, he reversed that inequality, suggesting that the number of channels be chosen based on how much computation is afforded (or on the needed resolution), and then truncating the phase function expansion at the same number of terms as the number of channels. According to Stamnes no systematic studies have been made to examine whether it would be useful to have more terms in the phase function expansion than the number of channels.

We suggest that the new SM-DORT model be implemented in MATLAB using the latest numerical software, in order to get a fast and stable solution of the eigenvalue problem. With the inverse problem in mind, stability and computational speed should be in focus.

Nevertheless, some effort should be made to keep the model modularised and easy to use, with a well-defined user interface. This will ensure that it will be easy to extend, and that scientists and industry can use it as a practical tool.

The inverse light scattering problem

Once a stable and fast model for the direct problem is present, the inverse problem will be the main concern. The characteristics of the inverse scattering problem need to be studied, in order to suggest an efficient parameter optimisation routine. This will include numerical implementation aspects such as determining derivatives efficiently (automatic differentiation) and choosing robust optimisation techniques. Methods for finding starting values for the optimisation routine should be investigated. The connection between measurements and
optimal parameters is very important and an analysis should be made in this direction. For example, it may be possible to perform measurements that will make the inverse problem more stable and easier to solve.

First, the inverse scattering problem needs to be formulated. The inverse problem will have different formulations and properties, depending on which direct model is chosen. Second, algorithms for the inverse problem need to be suggested and described. Third, experiments need to be designed and performed, in order to validate the results.

These steps will probably constitute an iterative process. For example, parameter dependencies might make it necessary to find a new set of parameters, which would change the direct model. The inverse problem will then need to be reformulated, and new experiments need to be designed in order to determine the parameters more easily and robustly.

**Experiments**

To evaluate the accuracy and predictability of a model, it must be tested against measurements. As described above, some experiments should be performed parallel to model simulations, and others to determine relevant parameters. Exactly which experiments need to be performed cannot be predicted in detail in advance, but some thoughts are given below, together with a short summary of available instruments.

**Experiments already performed**

There are many experiments done, measuring for example total reflectance and total transmittance, BSDF, gloss and more, that of course should be used to compare with model results.

An angle resolving model can be used to simulate light scattering distribution inside instruments, that otherwise do not allow for inspection, such as Elrepho 2000. This could yield corrections to instrument measurement errors due to instrument geometry, e.g. the gloss trap in Elrepho 2000.

**Suggestions for further experiments**

The most obvious experiments needed are, of course, angle resolved measurements of light scattering, to compare with the simulated results of SM-DORT, and to evaluate the physical relevance of the model and its parameters. Experiments should be done on both simple media with known physical properties, and on more complicated paper structures. It would be advantageous to cooperate with projects at Acreo and paper companies such as MoDo or SCA for experiments.
All models need as accurate physical parameters as possible. SM-DORT would need accurate values for the index of refraction for ingredients in a paper structure, for example ink, coatings and fibres.

In order to model rough surfaces, measurements are needed to give a qualitative description of surface roughness for different kinds of papers.

Knowledge is needed on how different media interact at boundaries when the media are not in perfect optical contact, or when different materials are mixed at the boundary. Are there thin intermediary layers? Is the optical contact homogeneously distributed, or are there islands with perfect and no optical contact respectively?

It would be interesting to know to what extent the asymmetry, scattering and absorption coefficients for a material is independent of each other, and how the coefficients change with respect to the wavelength of light.

Table 1. The following instruments can be used to measure light scattering from materials.

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Geometry</th>
<th>Lateral average</th>
<th>Spectrum</th>
<th>Where to find</th>
</tr>
</thead>
<tbody>
<tr>
<td>Datacolor Elrepho 2000</td>
<td>d/0</td>
<td>Ø 32 mm (variable)</td>
<td>16 bands visible, nonspectral selection of UV illumination</td>
<td>Most paper companies</td>
</tr>
<tr>
<td>Perkin-Elmer Spectrophotometer Lambda 19</td>
<td>8/d</td>
<td>~1×2 cm</td>
<td>More than 32 bands visible and UV detection</td>
<td>ACREO</td>
</tr>
<tr>
<td>Labsphere Bispectral Fluorescence Colorimeter BFC-450</td>
<td>45/0</td>
<td></td>
<td>32 bands visible, Double monochromator enables spectral UV illumination</td>
<td>Labsphere at MITATEN in Finland</td>
</tr>
<tr>
<td>ARS</td>
<td>Variable collimated illuminated detection and illumination</td>
<td>Ø 1.2 mm (depends on angle of incidence)</td>
<td>633 nm red light</td>
<td>ACREO</td>
</tr>
<tr>
<td>Densitometer</td>
<td></td>
<td></td>
<td>3 or more</td>
<td>Printing companies</td>
</tr>
<tr>
<td>Scanner</td>
<td></td>
<td>Laterally resolved image</td>
<td></td>
<td>Most companies</td>
</tr>
<tr>
<td>Camera</td>
<td></td>
<td>Laterally resolved image</td>
<td>Visible</td>
<td>Accurate camera at SCA</td>
</tr>
</tbody>
</table>
Figure 1. Angle-resolved measurement geometry according to ASTM:E1392-96.
Figure 2. Geometry of Lambda 19 and Elrepho 2000 instrument geometries.

The Elrepho 2000\textsuperscript{19,20} is thoroughly used in the paper industry to benchmark the optical quality of paper, e.g. color\textsuperscript{21}, opacity\textsuperscript{22}, and whiteness\textsuperscript{23}. The brightness of pulp, paper, and paperboard should according to TAPPI be measured with a 45/0 geometry instrument\textsuperscript{24}, but according to ISO\textsuperscript{25} with a d/0 geometry instrument.

Table 2. The instruments below can be used to measure the structure of materials.

<table>
<thead>
<tr>
<th>Measures</th>
<th>Information</th>
<th>Where to find</th>
</tr>
</thead>
<tbody>
<tr>
<td>Talystep</td>
<td>Surface profile</td>
<td>ACREO</td>
</tr>
<tr>
<td>AFM</td>
<td>Surface area</td>
<td>Mitthögskolan, ACREO</td>
</tr>
<tr>
<td>CLSM (confocal microscope)</td>
<td>Surface area</td>
<td>PFI in Norway</td>
</tr>
<tr>
<td>SEM</td>
<td>Surface area</td>
<td>SCA</td>
</tr>
<tr>
<td>Optical microscopes</td>
<td>Surface area</td>
<td>SCA, ACREO</td>
</tr>
<tr>
<td>Hg porosimetry</td>
<td>Bulk</td>
<td>SCA, MoDo</td>
</tr>
<tr>
<td>NMR</td>
<td>Bulk</td>
<td>YKI</td>
</tr>
<tr>
<td>ESCA</td>
<td>Surface</td>
<td>YKI</td>
</tr>
</tbody>
</table>
References


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   See also: ftp://climate.gsfc.nasa.gov/pub/wiscombe/Multiple_Scatt/

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