

# OPEN SOURCE MONTE CARLO SIMULATION PLATFORM FOR PARTICLE LEVEL SIMULATION OF LIGHT SCATTERING FROM GENERATED PAPER STRUCTURES

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**Abstract.** The Kubelka-Munk model and extensions thereof are extensively used in product development, thanks to their simplicity and the fact that they are invertible. However, their explanative power is limited to distinguishing processes that affect scattering properties from those that affect absorption properties, an example being the frequently observed decrease of the scattering coefficient with calendering. Better understanding of how internal structural changes affect the optical properties requires modelling the composite structure of a paper layer. We propose a modular object-oriented Open Source Monte Carlo simulation platform, *Open PaperOpt*, which allows different geometrical representations of the inner paper structure. The proposed file formats open for a standardisation that facilitates data exchange between different simulation tools and measuring instruments, and supports a broad dissemination of the simulation software. We applied the model to the analysis of the effect of calendering on the optical properties of uncoated paper. The simulation results agreed well with reflectance measurements and indicate that the light scattering decrease due to calendering can be explained by a change in pore size and shape.

**Keywords:** Light scattering, Monte Carlo simulation, Paper structure modelling

## 1 Introduction

Due to the lack of general solutions to the problem of multiple scattering by tightly packed particles, established light scattering models are based on phenomenological theories that describe paper as homogenous turbid layers. Thanks to their simplicity and the fact that they are invertible (enabling material constants to be directly determined from reflectance measurements), the Kubelka-Munk model and extensions thereof are still extensively used in product development and can successfully predict the reflectance of layered printed papers from the scattering and absorption properties of each layer. When it comes to process unit operations or layer mixtures, the models rely on additivity rules that are not always valid, and their explanative power is limited to distinguishing processes that affect the scattering properties from those that affect the absorption properties. One example is the frequently observed decrease of the scattering coefficient with

calendering [12]. Better understanding of how the internal structure affects the optical properties requires modelling the composite structure of a paper layer, which inevitably increases the model complexity.

Whenever the equations describing a physical problem can be written down, but the solution to these equations is intractable, it is appealing to turn to Monte-Carlo methods. By following the path of wave packets interacting with different components according to local physical rules, it is possible to calculate the average spatial- and angle resolved reflectance and transmittance. The method has been extensively used in medicine applications to model the interaction of light with tissues [14]. Carlsson *et al.* [2] introduced a three-dimensional model of the internal structure of paper including flattened cylindrical fibres, ellipsoidal pores, and fine particles located on the fibre surface that cause random anisotropic scattering. Hainzl *et al.* [6] proposed an extended implementation that includes rough surface scattering, layer thickness variation, and fluorescence. This statistical description of the paper structure, using component distributions and size distributions, does not render the structure of the a sheet, but it simulates the average optical response of the paper. Another approach is to use physical models of the structure of the fibre network. Light scattering simulation models using such generated paper structures were suggested by Niskanen [10] and Jensen [8] among others, and improved fibre web modelling has been published recently [4, 13].

Continued development of simulation models in an Open Source project opens for faster development and broader international collaboration. This paper introduces a novel open source Monte Carlo simulation tool for the modelling of light scattering in paper and prints. The program structure is described in Section 2 and selected physical models are presented in Section 3. The use of Monte Carlo simulation models is then discussed in Section 4 and illustrated in Section 5, where the effect of calendering on the optical properties of uncoated paper samples is analysed.

## 2 Structure of the simulation tool

The Monte Carlo scheme and the modular object-oriented design of the program allow different geometrical representations of the inner paper structure, and facilitate simulation of virtually any light source and detector. Paper layers with varying thickness and topography can be modelled as a turbid homogeneous material or as structural layers made of paper components such as fibres or filler aggregates. The layer structure can be either described statistically by means of material and geometrical distributions, or explicitly as a generated fibre network. The input parameters and output results are stored in a database of customised XML and HDF files, which opens for a standardisation that facilitates data exchange between different simulation tools and measuring instruments. The source code and a detailed description are available on the project website [11].

### 2.1 Implementation

The C++ program describes the paper as a three-dimensional layered structure. The thickness variation of each layer is controlled by delimiting surfaces, and the surrounding (e.g. air) is represented by the top and bottom layers of the simulated structure. Indivisible wave packets with initial direction, polarisation, and position defined by modifiable light sources are sent one at a time onto the top surface of the simulated structure, and

the following interaction is controlled by the chosen physical laws. All structure objects (surfaces and layers) send then the wave packet to the next object, until the wave packet leaves the simulated paper, or until it is absorbed without fluorescent re-emission. Different topographical representations of the surfaces are available. One specific surface representation uses a periodic dot structure to simulate halftone prints. Layers are made of components, which are geometric representations of the particles that build up the layer.

Two major classes of layers are implemented: static structural layers made of a fixed generated network of fibres, and statistical layers that simulate the composite structure statistically by generating components according to the layer's component distributions and the component geometric distributions. These structural layers combine to composite layers, and thus model light scattering from a system of geometric components such as hollow flattened cylinders and ellipsoids representing e.g. fibres, pigments, or pores.

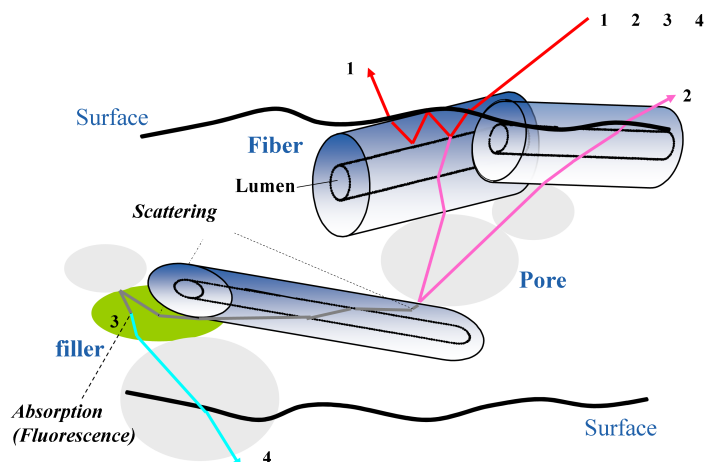
The simulation process is illustrated in Figure 1. In a statistical layer, the first component is given by the depth resolved component distribution of the layer. The size, shape, and orientation is then computed according to that component's geometric distributions. Each time the wave packet is about to leave the component, another component is generated and component surface scattering is computed. Wave packets can also be scattered, absorbed, or fluoresced within the component. In a static layer, the components' position and shape are well defined and fixed during the whole simulation, requiring generation of the 3D structure prior to the light scattering computations. Currently, only the network generation model proposed by Jensen [8], which is restrained to one type of fibre representation, has been implemented, but new network generation algorithms could easily be adapted to the internal data format of *Open PaperOpt*. The Monte Carlo simulation scheme makes extensive use of random number generators for specific distributions. All these distributions are organised in hierarchical classes in a specific namespace.

## 2.2 Data format

A detailed description of the paper structure together with the use of many different physical models lead to a tremendous amount of data. A database and a specific file format was therefore developed to structure the input parameters and simulated results. The details of the strategy adopted and the implementation are reported elsewhere [9].

All input specifications and results are stored in XML files, whose format is widely supported by numerous data analysis softwares. All parameters are marked up with a specific label and can easily be retrieved from files stored in the database. This allows searching for predefined components or layers and build paper structures from them. Low volume data such as the number of wave packets to be run are defined explicitly in the XML file, whereas large volume data such as topographies are stored in binary files or in the HDF standard (also widely supported). A description of the files is stored in the XML file, making the data retrievable from the database.

The proposed file format, which is part of the Open Source project, could be extended into a standard file format facilitating the exchange of data between different simulation tools and measurement instruments.



**Figure 1.** Examples of scattering processes in a structural layer. In a statistical description, all components are generated according to distributions, as the wave packet proceeds within the structure. In a static representation, the components have fixed positions. The path of a few wave packets is illustrated as follows: 1) enters the layer at the surface and is reflected after several bounces in a fibre; 2) bounces between fibres; 3) is absorbed in a filler aggregate; 4) is re-emitted at a longer wavelength (fluorescence) before it eventually leaves the paper structure in transmittance.

### 3 Light scattering simulation model

The modularity of the *Open PaperOpt* simulation tool allows implementing nearly any physical model for light scattering computations. Two fundamental steps are involved in setting up a simulation model. The first step is the geometric representation of the paper structure and its representation in terms of a statistical or static structure. The second step is to model the interaction of light with components in the layer. This interaction deals mainly with surface scattering at layer or component boundaries, and turbid medium scattering within parts of the components. This section presents the general underlying physical models used in the application presented in Section 5. Other geometric representations and physical models can easily be implemented by deriving new classes of layers or components, using existing ones as template.

#### 3.1 Surface scattering

Surface scattering is treated as a combination of two effects. The long-range topographic structure, called the surface waviness, is the part that deflects incident wave packets according to Snell's law and the Fresnel equations. In addition, the short-range topographic structure, called the microroughness, scatters the light diffusely. The scattering by the microroughness is introduced by letting a fraction of the reflected and refracted light be distributed in a Lambertian manner. For a surface with a Gaussian surface profile, the probability for diffuse scattering is given by Equation 1 for reflected light, and by Equation 2 for refracted light [1],

$$P_{\text{refl}} = 1 - e^{-\left(\frac{4\pi R_q n_i \cos \theta_i}{\lambda}\right)^2} \quad (1)$$

$$P_{\text{refr}} = 1 - e^{-\left(\frac{2\pi R_q n_i \cos \theta_i - n_t \cos \theta_t}{\lambda}\right)^2}, \quad (2)$$

where  $\lambda$  is the wavelength of the incident light,  $\theta_i$  is the incident angle,  $\theta_t$  is the refraction angle,  $R_q$  is the root mean square of the short-range topography, and  $n_i$  and  $n_t$  are the refractive indices of the media delimited by the surface. The polarisation state of the specularly reflected/refracted light is determined by the Fresnel equations. For the diffuse part, the polarisation state is determined by the Q-matrix [5].

### 3.2 Scattering, absorption, and fluorescence in a homogeneous turbid medium

Within a homogenous turbid medium representing e.g. a fibre wall, a filler aggregate or a whole layer, the scattering process is controlled by three parameters, the scattering and absorption coefficients,  $\sigma_s$  and  $\sigma_a$ , and the asymmetry factor  $g$ . The probability of travelling a distance  $t$  before a scattering or absorption event is given by

$$P(t) = (\sigma_s + \sigma_a)e^{-(\sigma_s + \sigma_a)t}. \quad (3)$$

If fluorescence is present, light can be re-emitted at a longer wavelength according to a fluorescence matrix defining the probability for absorption and emission at different wavelengths. Scattering distributions, such as the Henyey-Greenstein phase function [7] controlled by the asymmetry factor  $g$ , are used to compute the new direction of the wave packet after scattering. When  $g$  is zero, as in the application presented in this report, this distribution is uniform and the single scattering process is isotropic.

## 4 Using Monte Carlo light scattering simulations

Although simulation does not always aim at modelling or predicting real paper samples (it can be used for instance to estimate the effect of one parameter on a certain measurable quantity), its *validation* and *explanative power* rely on representing the investigated phenomena in such a manner that relevant conclusions can be drawn. Monte Carlo is not in itself a model of the light scattering properties of paper. In order to run a simulation, the particles building a paper layer, their distributions within the sheet, and the physical models of their interaction with light must be represented by parameterised functions, whose parameters are then determined by direct or indirect measurements (parameter estimation). In the Kubelka-Munk (KM) theory, the situation is much simpler, and standardised methods relate directly the model parameters to a pair of reflectance measurements. On the other hand, a Kubelka-Munk based model makes use of assumptions to simplify the paper structure representation to such an extent that no structure information is left. Moreover, the KM parameters do not have any physical meaning outside the KM theory. Any model will nonetheless rely on simplifications and assumptions. These have to be chosen so that the relevant structural information related to the phenomenon under investigation is preserved. In some cases, modelling a layer as a homogeneous scattering layer will be sufficient, if only thickness variation and angle-resolved scattering are properly considered.

The choice of representation of the simulated structure, whether it is a statistical or a generated static representation, results in a number of parameters to be determined. Further simplifications might then be used to assume some parameters, e.g. assuming the

fibre wall thickness to be a constant ratio of the fiber width. The other parameters are model parameters. The *applicability* of the model then relies on available measurement methods to determine these parameters. Some parameters cannot be measured directly but are instead determined via optimisation of the parameters to fit simulated values to measured ones. A measure of *robustness* of the model is then how well these optimised parameters can be used in other simulations. This includes physical parameters such as the fibre surface microroughness and the absorption coefficient in the fibre wall.

The model has to be defined so that the optimisation problem is not underdetermined, since this would lead to several solutions that are only valid for the set of samples used for the parameter estimation. Other measurable quantities that are not directly related to light scattering must also be taken into account for model *consistency*. This includes for instance the basis weight of a simulated sheet that must be constant regardless of the particle size distributions and sheet thickness. Using a Markov chain formalism, Dahlgren [3] developed an analytical determination of the basis weight from the components' size distributions and density, which can be used to control the basis weight of the simulated sheet.

## 5 Application to the reflectance from uncalendered and calendered sheets

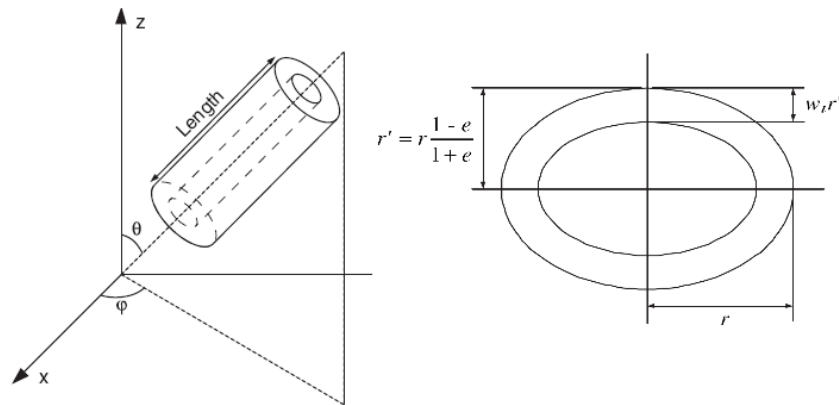
This section illustrates the method described above. *Open PaperOpt* was used to model the light scattering from uncalendered and calendered sheets to study the reported decrease of the reflectance factor with calendering [12].

### 5.1 Paper samples

Sheets of eucalyptus and pine pulp were prepared at three basis weights with a Formette Dynamique at a speed of 1200 rpm and a pump pressure of 4.2 bar. These parameters are optimised to get the lowest anisotropy in the sheets. Thereafter the sheets were pressed five minutes in a Lorentzen & Wettre sheet press at a pressure of 0.6 MPa. Finally, the sheets were dried in an STFI oven up to a temperature of 88 °C. Thirty sheets of each pulp type and basis weight were prepared, of which half were calendered twice on each side at a temperature of 100 °C and a pressure of 160 bar.

### 5.2 Characterisation: Model design and assumptions

Each sheet was modelled as a statistical layer bounded by two flat surfaces, simulating a sheet with constant thickness. Fibres were modelled as rough hollow cylinders, stretched out into an elliptic shape defined by the polar angle of the fibre direction ( $\theta$ ), the azimuthal angle ( $\varphi$ ), the length of the fibre ( $l$ ), the fiber radius ( $r$ ), the relative thickness of the fiber wall compared to the minor axis of the elliptic cross-section ( $w_t$ ), and the cross-section ellipticity ( $e$ ) (Figure 2). The fibres were assumed to be homogeneously distributed along the thickness direction of the sheet and isotropically oriented in the plane of the paper ( $\theta = 90^\circ$ ). Pores were modelled as flattened spheres defined by a radius distribution and a fixed cross-section ellipticity. Fibre contact was neglected, the porosity at the sheet surface was set to 50%, and no scattering in the fibre wall was allowed. Thus, the only contribution to light scattering came from light reflections at fibre and layer boundaries. The refractive index of the layer and fibre wall was set to 1.5

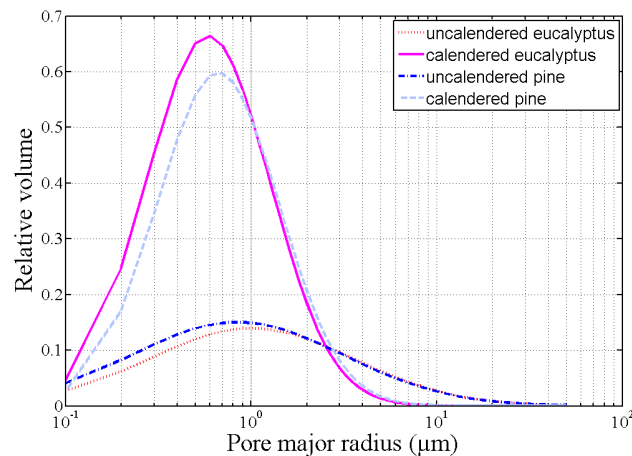


**Figure 2.** The geometric layout of a fibre.

and the fibre wall density was set to  $1.65 \text{ kg/dm}^3$ .

### 5.3 Characterisation: Measurements

The sheet thickness was measured with a STFI-thickness tester. The fibre length and width distributions were obtained from FiberMaster measurements. The pore size distribution of the sheets was estimated using mercury porosimetry. The measured distributions were then fitted against a log-normal distribution for each sheet type. The same distributions were used for all sheet basis weights. The fitted distributions are shown in Figure 3.



**Figure 3.** Estimated pore size distribution for the uncalendered and calendered pine and eucalyptus sheets.

### 5.4 Characterisation: Parameter estimation

Having defined the size distribution of the pores and fibres and the fibre wall density, the basis weight of the simulated fibre network is determined by the fibre wall thickness and the fibre and pore ellipticities. The fibre ellipticity was estimated to 0.3 for eucalyptus and 0.4 for pine from analysis of SEM cross-section images. The fibre wall thickness parameter and the pore ellipticity were optimised to best fit the nominal basis weights of

the three uncalendered sheets. For the calendered sheets, the same fibre geometry was kept and a new pore ellipticity was determined. Finally, the fibre surface microroughness and the cellulose light absorption were determined by fitting the simulated reflectance of the 60 g/m<sup>2</sup> uncalendered sheets and of an opaque pad of uncalendered sheets to the measured reflectances. The parameters used in the simulations are given in Table 1.

**Table 1.** The optimised pore ellipticity, fibre wall thickness parameter, fibre surface microroughness, and light absorption coefficient in the fibre wall for the two types of pulp, eucalyptus (E) and pine (P). The measured sheet thicknesses for both the three calendered (cal) and the three uncalendered (unc) samples are tabulated in the last row.

Sample	E. Cal.	E. Unc.	P. Cal	P. Unc.
$e_{pore}$	0.74	0.06	0.9	0.05
$w_{fibre}$	0.42	0.42	0.42	0.42
$R_q(\mu m)$	0.06	0.06	0.05	0.05
Fibre $\sigma_a(\mu m)$	5e-6	5e-6	5e-6	5e-6
Thickness ( $\mu m$ )	64-105-130	125-204-270	67-100-135	116-188-253

## 5.5 Results

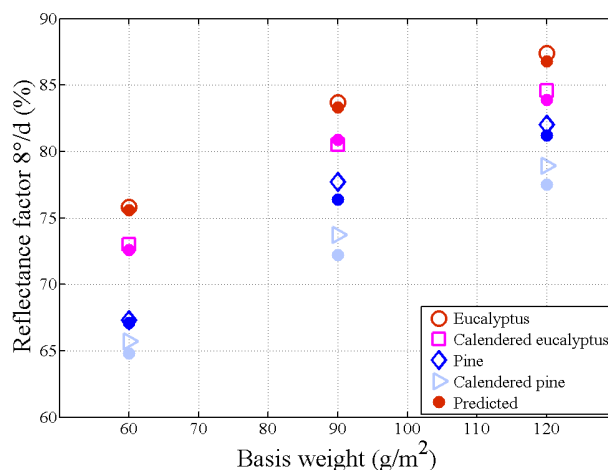
The simulation results are in Figure 4 compared to measured reflectances obtained with an 8°/d Perkin Elemer Lambda 19 spectrophotometer. The simulated reflectance of the 60 g/m<sup>2</sup> uncalendered pine and eucalyptus sheets were fitted to the corresponding measured reflectances in order to optimise the fibre surface microroughness and the absorption coefficient in the fibre wall. We assumed that the fibres are not affected by the calendering process and neglected fibre contact in both calendered and uncalendered sheets. For the calendered sheets, only the pore size and ellipticity were adjusted to compensate for the sheet thickness decrease and density increase.

The simulated reflectances at higher basis weight agreed fairly well with the experimental ones. For the calendered sheets, the simulated reflectance values followed the decrease in the measured reflectance. This indicates that the observed reflectance decrease due to the calendering process can be explained by a change in pore size and shape.

## 6 Conclusions and suggestions for further work

Given the complexity of the composite paper structure, modelling of the optical properties requires simplifications, but the Kubelka-Munk model makes assumptions to such an extent that no structure information remains. Hence, its explanative power is limited to distinguish processes that affect its phenomenological scattering parameter from those that affect the corresponding absorption parameter. Better understanding the how the internal structure affects the optical properties requires a model that preserves the structural information related to the phenomenon under investigation. The exact modelling of the interaction of light with such structures is however intractable, and therefore Monte Carlo simulations are employed.





**Figure 4.** Experimental and simulated  $8^\circ/d$  total reflectance factor. The fibre surface micro-roughness and the absorption within the fibre wall were optimised to fit the reflectance factor of the  $60 \text{ g/m}^2$  uncalendered sheets. The reflectance factor was then predicted for the  $90 \text{ g/m}^2$  and  $120 \text{ g/m}^2$  sheets and for all three calendered sheets. The pore size distribution was measured before and after calendering, and the pore ellipticity was adjusted to fit the actual sheet thickness. Open markers are the measurements and the corresponding points are the simulated values. The observed reflectance decrease is predicted by a change in pore size and shape.

We presented an Open Source Monte Carlo simulation tool, *Open PaperOpt*, which allows different geometrical representations of the paper structure and different physical models of their interaction with light. The paper structure can be represented statistically with component distributions, or by a generated fibre network. The applicability of the simulation tool was demonstrated by modelling the effect of a structure modification on the light scattering. The results indicated that the decrease in light scattering due to calendering can be explained by a change of pore size and shape, all else being equal.

The current version of *Open PaperOpt* is a modular extension of existing models previously implemented separately. Specific XML based file formats were implemented and a database was developed to search for and save simulation input and output. The proposed file formats open for a standardisation that facilitates data exchange between simulation tools and measurements. Being an Open Source project, the proposed simulation platform supports faster future development of simulation models and a broader dissemination of the results. Contributions from the scientific community are highly encouraged, and will pave the way for a standard simulation platform specific to the paper industry. Future work, which is not restrained to paper optics, includes enhanced physical models (e.g. fluorescence related), and 3D paper generators that could be extended to represent fillers and coating.

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