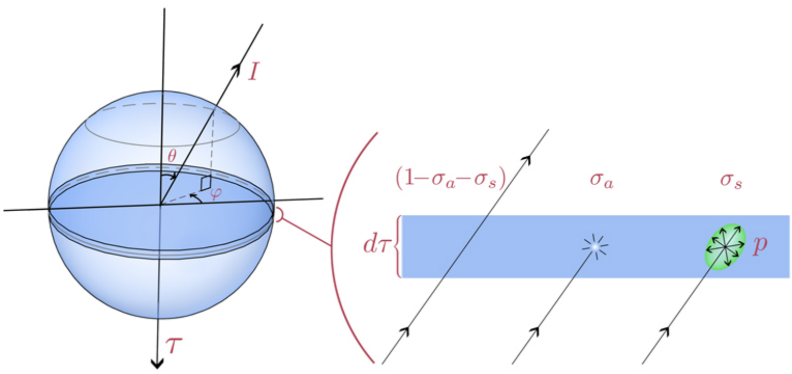
Mathematical Modelling of Light Scattering in Paper and Print

Per Edström



$$u\frac{dI(\tau,u,\varphi)}{d\tau} = I(\tau,u,\varphi) - \frac{a}{4\pi}\int_0^{2\pi}\int_{-1}^{1} p(u',\varphi';u,\varphi)I(\tau,u',\varphi')du'd\varphi'$$

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Abstract

A problem formulation and a solution method are outlined for the radiative transfer problem in vertically inhomogeneous scattering and absorbing media, using discrete ordinate model geometry. The treatment spans from the physical problem via a continuous formulation, a discretization and a numerical analysis, to an implementation with performance evaluation and application to real-world problems. The thesis clearly illustrates how considerations in one step affect other steps, and thus provides an example of an overall treatment of mathematical modeling of a large applied problem.

A selection of different steps is brought together. First all the steps necessary to get a numerically stable solution procedure are treated, and then methods are introduced to increase the speed by a factor of several thousand. The solution procedure is implemented in MATLAB under the name of DORT2002, and is adapted primarily to light scattering simulations in paper and print. A confined presentation is given of the effect of the steps that are needed, or possible, to make *any* discrete ordinate radiative transfer solution method numerically efficient. This is done through studies of the numerical performance of DORT2002.

Performance tests show that the steps that are included to improve stability and speed of DORT2002 are very successful. Together they give an unconditionally stable solution method to a problem previously considered numerically intractable, and decrease computation time compared to a naive implementation with a factor of 1 000 – 10 000 in typical cases and with a factor up to and beyond 10 000 000 in extreme cases. It is also shown that the speed increasing steps are not introduced at the cost of reduced accuracy, and that DORT2002 converges to the true value as the discretization is made finer.

It is shown by the use of DORT2002 that when a medium has a finite thickness, the light distribution deviates from the perfectly diffuse even under the theoretically ideal conditions for which the Kubelka-Munk model was created. This effect, which is in opposition to what one would intuitively expect, is caused by light escaping through the lower boundary of the medium, and causes errors in Kubelka-Munk reflectance calculations that can be up to 20% and more, even for a grammage of 80 g/m^2. The magnitude of the error shows a strong dependence on the degree of absorption, with higher absorption giving greater error. This confirms previously reported problems with Kubelka-Munk for strongly absorbing media, and DORT2002 offers a partial explanation of these problems, as it can describe this effect and quantify the Kubelka-Munk errors. It is argued that DORT2002 could well be considered for increased understanding in cases where the level of accuracy of Kubelka-Munk reflectance calculations is not acceptable. A comprehensive list of advantages for the applied user of a model with higher dimensionality is supplied.

Keywords: mathematical modeling; radiative transfer; solution method; numerical stability; speed; light scattering; light absorption; Kubelka-Munk; errors; reflectance calculations.

Svensk sammanfattning

En problemformulering och en lösningsmetod med discrete ordinate modellgeometri presenteras för radiative transfer problemet i vertikalt inhomogena spridande och absorberande material. Behandlingen spänner från det fysikaliska problemet över kontinuerlig formulering, diskretisering och numerisk analys, till implementation med prestandautvärdering och tillämpning på verkliga problem. Denna avhandling illustrerar tydligt hur överväganden i ett steg påverkar andra steg, och utgör därmed ett exempel på helhetsgreppet i matematisk modellering av ett stort tillämpat problem.

En mängd olika steg förs samman. Först behandlas alla steg som krävs för att få en numeriskt stabil lösningsmetod, och sedan introduceras metoder för att öka beräkningshastigheten med en faktor på flera tusen. Lösningsmetoden är implementerad i MATLAB under namnet DORT2002, och är främst anpassad till simulering av ljusspridning i papper och tryck. En sammanhållen presentation ges av effekterna av de steg som är nödvändiga eller möjliga för att göra *varje* discrete ordinate lösningsmetod till radiative transfer problemet numeriskt effektiv. Detta görs genom studier av numeriska prestanda hos DORT2002.

Prestandatester visar att de steg som inkluderats för att förbättra stabilitet och beräkningshastighet hos DORT2002 är mycket lyckade. Tillsammans ger de en ovillkorligt stabil lösningsmetod till ett problem som tidigare betraktats som numeriskt ohanterligt, och minskar beräkningstiden jämfört med en naiv implementation med en faktor 1 000 – 10 000 i typiska fall och med en faktor upp till och över 10 000 000 i extremfall. Det visas också att stegen för att öka beräkningshastigheten inte introducerats på bekostnad av reducerad noggrannhet, och att DORT2002 konvergerar mot det riktiga värdet när diskretiseringen görs finare.

Det visas genom användning av DORT2002 att när ett medium har ändlig tjocklek avviker ljusdistributionen från den perfekt diffusa även under de teoretiskt ideala förhållanden som Kubelka-Munk modellen skapats för. Denna effekt, som motsäger vad man intuitivt skulle vänta sig, uppstår genom att ljus försvinner genom mediets nedre rand, och orsakar fel i reflektansberäkningar med Kubelka-Munk som kan vara upp till 20% eller mer, även för ytvikter på 80 g/m^2. Storleken på felet uppvisar ett starkt beroende på graden av absorption, där högre absorption ger större fel. Detta bekräftar tidigare rapporterade problem med Kubelka-Munk för starkt absorberande medier, och DORT2002 ger en delförklaring till dessa problem eftersom den kan beskriva denna effekt och kvantifiera felen i Kubelka-Munk. Det argumenteras att DORT2002 kan övervägas för ökad förståelse i fall där noggrannheten för reflektansberäkningar med Kubelka-Munk inte är tillräcklig. Fördelar med modeller av högre ordning för tillämpade användare beskrivs i en omfattande lista.

Front cover. Radiative transfer in a nutshell.

Top left. The coordinate system used, where the Cartesian coordinate τ is the optical depth, and the angular coordinates θ and φ from spherical geometry designate the direction of propagation of a beam of radiation with the intensity I.

Top right. Enlarged image of a layer of the infinitesimal thickness $d\tau$. The relative probabilities of transmission, absorption and scattering upon passage of the layer are $1 - \sigma_a - \sigma_s$, σ_a and σ_s, respectively, where σ_a and σ_s are the absorption and scattering coefficients. The phase function p specifies the probability distribution of different scattering directions.

Bottom. The fundamental integro-differential equation of radiative transfer, where $u = \cos\theta$, and $a = \sigma_s / (\sigma_a + \sigma_s)$. This thesis is about solving this equation, and applying it to light scattering in paper and print.

List of Papers

This thesis is based on the following papers, herein referred to by their respective Roman numerals.

Paper I **A Fast and Stable Solution Method for the Radiative Transfer Problem**
Edström, P.
To be published in *SIAM Review* (2005).

Paper II **Numerical Performance of the DORT2002 Radiative Transfer Solution Method**
Edström, P.
Submitted to *Applied Numerical Mathematics* (2004).

Paper III **Comparison of the DORT2002 Radiative Transfer Solution Method and the Kubelka-Munk Model**
Edström, P.
Published in *Nordic Pulp and Paper Research Journal* 19(3), pp 397-403 (2004).

Paper IV **Quantification of the Intrinsic Error of the Kubelka-Munk Model Caused by Strong Light Absorption**
Granberg, H. and Edström, P.
Published in *Journal of Pulp and Paper Science* 29(11), pp 386-390 (2003).

Table of Contents

1. Introduction

This thesis is about mathematical modeling, and it treats all steps from a physical process to a practical tool for an applied user. One overall purpose of this thesis is to go through all these steps for a large applied problem, and thus illustrate how considerations in one step affect other steps. Most papers on mathematics treat a specialized part of a larger problem, but when it comes to solving large applied problems, it is not as simple as picking solutions for given sub-problems and combining them. Naturally, since most papers are so specialized, such issues are seldom treated. This thesis contributes to applied mathematics by being in itself an extensive example of this overall treatment.

This thesis is also about light scattering in paper and print. The overall goal of this aspect of the thesis is to develop an improved model for light scattering in paper and print, to facilitate faster and more accurate simulations and measurement methods. This has been done in two simultaneous parts. One part has been to investigate the more general radiative transfer problem in a broad manner, and to combine chosen parts of different solution methods from the various application areas with ideas from modern scientific computing. The other part has been to learn the needs of the paper and printing industry by taking part in several applied projects, and finally also by contributing to them. The entry points to these projects, conducted in academia, at institutes and in the industry, have been through the networks FSCN (Fibre Science and Communication Network, at the Mid Sweden University) and T2F ("TryckTeknisk Forskning", a Swedish printing research program). This thesis contributes to the area of light scattering in paper and print by providing the DORT2002 model.

2. Radiative Transfer

Radiative transfer theory describes the interaction of radiation with scattering and absorbing media. It has been applied to such different applications as stellar atmospheres, infrared and visible light in space and in the atmosphere, optical tomography and diffusion of neutrons. An industrially important application is light scattering in textile, paint, pigment films, paper and print, and accurate calculation methods are crucial for these sectors of industry.

Discrete ordinate solution methods for radiative transfer problems have been studied throughout the last century. In the beginning most radiative transfer problems were considered intractable because of numerical difficulties. Therefore coarse approximations were used, and methods developed slowly due to the lack of mathematical tools. As computers have become faster and more readily available, highly efficient and specialized solution methods have been developed. Among the solution methods in use today are discrete ordinate methods, methods using spherical harmonics, methods using finite elements or finite differences, and Monte-Carlo methods.

The first approximate solution to the radiative transfer problem was presented by Schuster [1], who considered only diffuse radiation, and exclusively in a forward and a backward direction. Clearly influenced by this, Kubelka and Munk [2] developed their well-known model, which was further refined by Kubelka [3, 4]. The models presented by Schuster and Kubelka and Munk, and others after them, are known as two-flux models.

By using numerical quadrature to approximate an integral with a finite sum, Wick [5] gave the first general treatment of discrete ordinate methods for the radiative transfer problem. The terms in the sum can be interpreted as the contribution to flux or intensity from a discrete cone in spherical geometry. The polar angles of these cones are referred to as discrete ordinates, which has given the method its name, and the cones are called channels or streams. Using only two channels gives the earlier two-flux methods. If more channels are used, the methods are referred to as multi-flux methods or many-flux methods. Chandrasekhar [6] described a method using spherical harmonics, but having read Wick's article, he adopted the discrete ordinate method, and further refined it [7]. Later, he wrote a classic exposition on radiative transfer theory in book form [8], and since then the area has expanded tremendously.

Mudgett and Richards [9, 10] described a discrete ordinate method for use in technology, and reported on numerical difficulties, as have many before and after them. These difficulties worsened when the use of computers made it possible to tackle larger problems. Only when recognizing the numerical difficulties can measures be taken to avoid unstable algorithms and ill-conditioned problems. A careful analysis of the problem makes it possible to find such measures, and advances in numerical linear algebra and scientific computing provide ideas and software tools to make it a tractable problem. A number of such issues are, among plenty of applied physics, addressed in a recent textbook on radiative transfer in the atmosphere by Thomas and Stamnes [11].

3. Light Scattering in Paper and Print

There is an obvious need for optical modeling in the paper industry for printing papers with increased demands for the "right appearance". This need is also driven by increasing competition from other media. The modeling would provide connections between the actual properties of the paper products and their perceived optical quality. Indeed, the appearance of paper products is also becoming increasingly important in the field of packaging and hygiene products, where the "right impression" also includes the appearance of the product.

Examples of areas where optical modeling is used within the paper industry are fine-tuning the papermaking process, designing new paper qualities, color management from pre-press to print, and evaluating printing techniques. Today the Kubelka-Munk model (or extended models thereof) is most widely used to cover these applications. As is well known, the Kubelka-Munk light scattering and light absorption coefficients (s and k) are extensively used in the pulp and paper industry in applications ranging from research projects to practical problems in paper mills. Examples are prediction of brightness and opacity of papers containing different pulps and fillers, or papers with multilayer structures (coated and printed papers). These coefficients provide a link between the (measured) reflectance factor, e.g. brightness, and properties of the paper sample, so that the reasons for a high or low reflectance can be better understood. The *s* and *k* values are also linked to unit operations in pulp and paper technology through many investigations over the years. The reasons for this extensive use of the Kubelka-Munk model are most likely the simplicity of the equations (which was a major advantage before the introduction of personal computers) and the fact that they are invertible, roughly meaning that reflectance values can be calculated from *s* and *k*, and that *s* and *k* can be calculated from reflectance values.

When Kubelka and Munk presented their model, it was state-of-the-art, but now it should be seen as the approximation it is. Several limitations for the Kubelka-Munk model have been reported, for example concerning dependencies between the *s* and *k* coefficients for translucent or strongly absorbing media [12-15], and attempts have been made to attribute some of this behavior to intrinsic errors of – or phenomena not included in – the Kubelka-Munk model [16-19]. Despite these limitations, the Kubelka-Munk model is in widespread use for multiple scattering calculations in paper, paper coatings, printed paper, paint, plastic and textile, probably due to its explicit form and ease of use. These are also reasons for continued usage where the accuracy is sufficient, and where there are no reported limitations. However, new solution methods with better accuracy and a larger range of applicability should be considered in many cases. Given the fast development of personal computers, it is well worth investigating other solution methods that give a more detailed and more accurate description of the paper sample, and yet can easily be made accessible for the applied user. It is argued in this thesis that the DORT2002 model presented herein can well be considered for increased understanding in cases where the level of accuracy of Kubelka-Munk reflectance calculations is not acceptable. Indeed, DORT2002 is already in use in a number of research projects.

4. Summary of the Papers

The papers that this thesis is based on together follow a natural line in mathematical modeling of light scattering in paper and print, going from a physical problem to a practical tool for an applied user. Paper I states a problem formulation and achieves an effective solution method, DORT2002. Paper II presents an evaluation of the numerical performance of an implementation of DORT2002. Papers III and IV use DORT2002 to identify and quantify errors of Kubelka-Munk, and offer it as a tool in future research.

4.1. Paper I

This paper starts with the problem of scattering and absorption of radiation in multilayer turbid media, and formulates it as a radiative transfer problem. The solution method is carried as far as possible in a continuous formulation before it is discretized. It is then numerically analyzed, and all numerical difficulties, such as ill-conditioning and slowness, are overcome by using knowledge from the continuous formulation and the underlying physics. A selection of different steps is brought together. First all necessary steps to get a numerically stable solution procedure are treated, and then methods are introduced to increase the speed by a factor of several thousand. DORT2002 is implemented in MATLAB, and is adapted primarily to light scattering simulations in paper and print. Its task is to calculate the light intensity in any direction and at any depth inside and outside an illuminated medium, but also to calculate quantities derived from the intensity such as bidirectional scattering distribution function (BSDF), total reflectance, total transmittance, total absorptance and flux.

DORT2002 uses expansion in Legendre functions, and then Fourier analysis on the azimuthal angle variable, to turn an integro-differential equation into a number of uncoupled equations. These equations, one for each Fourier component of the unknown intensity, are then discretized using a specialized Double Gauss numerical quadrature. This yields a system of first order linear differential equations for each layer in each Fourier component, and the customary solution procedure gives an eigenvalue problem. The situation with boundary and continuity conditions is treated, as well as the problem of extending the computed intensity from the quadrature points to the entire interval by creating interpolation formulas. The flowchart below describes the overall structure of DORT2002.

```
for  all Fourier components
     for  all layers
          Solve system of ODE:s through an eigenvalue problem.
          Represent homogenous solution by a linear combination of the
          eigensolutions with (so far unknown) coefficients.
          Compute particular solution.
     end
     Apply boundary and continuity conditions to obtain the unknown
     coefficients of the homogenous solution.
     if   convergence criterion is met
          Break loop over Fourier components.
     end
end
Assemble total intensity as sum of Fourier components.
Apply interpolation formulas.
```

DORT2002 includes several steps that improve stability. Some of them have an obvious effect in a limited part of the method. Among these are the following; the numerically stable way of evaluating normalized associated Legendre functions, the fast and numerically stable method adapted to find nodes and weights for the Double Gauss quadrature formula that is optimal for this specific problem, the interpolation formulas expressed in the solutions of the eigenvalue problems, and finally the avoidance of overflow and divide-by-zero situations. The step that has the most profound influence on the stability of the overall method is the preconditioning of the system of equations corresponding to the boundary and continuity conditions.

Several steps are included to increase the speed of DORT2002. Among these steps are the great effort made to handle and exploit the sparse structure of the systems of equations corresponding to the boundary and continuity conditions, and code optimization using known programming principles for MATLAB. Other steps have a more profound influence on the speed of the overall method. These include the eigenvalue problem size reduction, methods that maintain accuracy for a coarser discretization, and methods that terminate calculations on earlier convergence.

4.2. Paper II

This paper studies the numerical performance of DORT2002, in terms of stability, speed and accuracy. The focus is on the effects of the steps that are needed to make the method numerically efficient, and the steps that differ from a naive implementation. The point of this paper is not to describe the best possible solution method for the radiative transfer problem; the field is so diverse that specialized routines are needed that exploit the special properties of each specific application area. Instead, the point is to give a confined presentation of the effect of the steps that are needed, or possible, to make *any* discrete ordinate radiative transfer solution method numerically efficient, and specifically the effect of all the major steps included in DORT2002 that are described in Paper I. The resulting improvements, quantified in terms of reduced condition number and increased speed compared to a naive implementation, are illustrated.

Performance tests show that the steps that are included to improve stability and speed of DORT2002 are very successful. Together they give an unconditionally stable solution method to a problem previously considered numerically intractable, and decrease computation time compared to a naive implementation with a factor of 1 000 – 10 000 in typical cases and with a factor up to and beyond 10 000 000 in extreme cases. It is also shown that the speed increasing steps are not introduced at the cost of reduced accuracy, and that DORT2002 converges to the true value as the discretization is made finer.

4.3. Paper III

The purpose of this paper is to draw attention to the potential of models of higher dimensionality for optical modeling of paper, since modern computers make it fully tractable to use such models. It is argued that modern solution methods from radiative transfer theory could be considered instead of the Kubelka-Munk model to provide connections between the optical response of a paper and its actual properties. In this paper, DORT2002 is used as an example of such models.

It is shown that Kubelka-Munk, which is the predominantly used model in paper and print applications today, is a simple special case of DORT2002, or conversely that DORT2002 is a true generalization of Kubelka-Munk, and not just another extension. An exact translation between the coefficients of the Kubelka-Munk and the DORT2002 models is shown to be valid under the conditions of perfectly diffuse light, perfectly isotropic scattering, and only two channels in the DORT2002 model. Under these conditions it is shown to hold that $s = \sigma_s$ and $k = 2\sigma_a$, where σ_s and σ_a are the scattering and absorption coefficients of DORT2002. Since Kubelka-Munk is a simple special case of DORT2002, all previous knowledge such as tables, parameter values, measurements etc can still be used, so nothing needs to be discarded. On the contrary, it provides a strong foundation for future work with both models.

It is shown that when the medium has finite thickness, the light distribution deviates from the perfectly diffuse even if illumination and scattering are perfectly diffuse, which is in opposition to what one would intuitively expect. This effect is caused by light escaping through the lower boundary of the medium, and causes errors in Kubelka-Munk reflectance calculations that can be up to 20% and more, even for a grammage of 80 g/m^2. The magnitude of the error shows a strong dependence on the degree of absorption, with higher absorption giving greater error. This confirms previously reported problems with Kubelka-Munk for strongly absorbing media [12-15], and DORT2002 offers a partial explanation of these problems, as it can describe this effect and quantify the Kubelka-Munk errors. Cases with large errors are not infrequent in practice, but include cases such as heavily dyed papers or full tone prints. It is discussed that since Kubelka-Munk is often used in a self-consistent manner, the errors may cancel to a varying extent, and will not always be apparent. The errors are most likely to be visible if s and k are determined for samples of a certain grammage, and then applied to predict reflectances for a sample of a different total grammage. Further investigation is needed to establish what this implies for the application of the Kubelka-Munk model.

From the point of view of the applied user, angle-resolved models such as DORT2002 have several advantages compared to the Kubelka-Munk model. The angular distribution of reflection and transmission can be modeled, as well as different scattering asymmetries of the bulk. Collimated light can be used to analyze the optical response of a sample, while the Kubelka-Munk model is limited to diffuse light. Since any illumination and detection conditions can be handled, the interior of instruments otherwise closed for inspection can be simulated, and the influence of instrument geometry on measurements can be evaluated. This makes it possible to suggest measurement corrections for deviations due to instrument geometry, and to make calibration and measurements with different instrument geometries comparable. Furthermore, DORT2002 is consistent for translucent and highly absorbing media, and is prepared to be combined with a surface model to handle gloss. It is also prepared for a future implementation of fluorescence, which will allow the effect of OBA (optical brightening agents) in paper and print to be modeled. This opens the field for finding new connections between the properties of paper and its perceived optical quality. The whiteness and brightness of paper cannot be designed with the Kubelka-Munk model since fluorescence phenomena are not explicitly included.

4.4. Paper IV

In this paper, intrinsic errors of the Kubelka-Munk model are mapped by comparing light-scattering calculations from the Kubelka-Munk model with the more accurate model DORT2002. Comparisons are made with previous experimental observations, and it is found that intrinsic errors in the Kubelka-Munk model explain around 20% of the previously observed interdependence of the Kubelka-Munk coefficients for heavily dyed sheets. It is argued that an even greater percentage can be explained by taking into account light scattering and internal reflectance from a rough top surface, and the geometry of the optical instrument used in the measurements, and models that account for this are called for.

5. Contribution of the Thesis

One overall contribution of this thesis is to treat a large applied problem, go through all steps from a physical process to a practical tool for an applied user, and thus illustrate how considerations in one step affect other steps. Most papers on mathematics treat specialized parts of large problems, and rightfully so – they represent advances in their respective field, and give hints for further research and provide knowledge for others to use. But when it comes to solving large applied problems, it is not as simple as picking solutions for given sub-problems and combining them. Naturally, since most papers are so specialized, such issues are seldom treated. In fact, to be able to successfully synthesize solution methods from several different fields, a great depth of knowledge is often required in all these fields as well as in the physical background and in the final application area. This thesis contributes to applied mathematics by being in itself an extensive example of this overall treatment.

Another overall goal of this thesis is to develop a model, which improves on Kubelka-Munk, for light scattering in paper and print, to facilitate faster and more accurate simulations and measurement methods. This thesis contributes to the area of light scattering in paper and print by providing the findings in Papers III and IV, but also – and more important – by providing the DORT2002 model as an accessible tool for further investigations in the area.

5.1. Paper I

This paper goes through the steps from the problem of scattering and absorption of radiation in turbid media via a continuous formulation, a discretization and a numerical analysis, to implementation. A selection of different steps is brought together. The main contribution of the paper is the synthesis of these steps, all of which have been used in different areas, but never all together in one method. The paper provides several examples of how the solution of a sub-problem is facilitated by previous choices. For example, it is obvious how certain choices concerning the phase function and the numerical quadrature make it possible to reduce the size of eigenvalue problems several steps later. Another example is how the choice of problem formulation affects the possibility of finding a preconditioner for a system of equations. Only by starting with a continuous formulation could the elements in the coefficient matrix be known symbolically, thus allowing the construction of a preconditioner that is guaranteed to work. For several decades, solution methods of this type were discarded as numerically intractable due to the ill-conditioning of this system of equations. No general preconditioner could be constructed, because of the choice of starting with a discrete problem formulation. There is an intuitive geometrical interpretation of this kind of model geometry that light is scattered between discrete “channels”, which leads to an equivalent mathematical problem. But there the matrix elements are unknown transfer coefficients; they are not known symbolically, and neither are their relative sizes. The tempting choice of starting with a discrete problem formulation thus effectively held back advance in that area for decades.

5.2. Paper II

This paper gives a confined presentation of the effect of the steps that are needed, or possible, to make *any* discrete ordinate radiative transfer solution method numerically efficient. To the author's knowledge, this has not been summarized in one single publication before. This is done through studies of the numerical performance of the stability and speed increasing steps included in DORT2002.

5.3. Paper III

This paper shows, by the use of DORT2002, that when a medium has finite thickness, the light distribution deviates from the perfectly diffuse even under the theoretically ideal conditions for which the Kubelka-Munk model was created. This effect causes errors in Kubelka-Munk reflectance calculations that can be up to 20% and more, even for a grammage of 80 g/m^2. The magnitude of the error shows a strong dependence on the degree of absorption, with higher absorption giving greater error. It is argued that DORT2002 could well be considered for increased understanding in cases where the level of accuracy of Kubelka-Munk reflectance calculations is not acceptable. A comprehensive list of advantages for the applied user of a model with higher dimensionality is supplied.

5.4. Paper IV

This paper was the result of a cooperation with Dr Hjalmar Granberg. The contribution of the author of this thesis was to develop and supply DORT2002, and to perform and interpret the simulations, while the reasoning within applied paper optics is mainly Granberg’s. This paper gives a partial explanation of the previously observed interdependence of the Kubelka-Munk coefficients for heavily dyed sheets.

6. Some Practical Comparisons Between Kubelka-Munk and DORT2002

It is worth saying something about absolute calculation times. DORT2002 is optimized for much larger and more complicated problems, and does much unnecessary work for the Kubelka-Munk case. Calculating total reflectance with Kubelka-Munk on a standard PC takes around 40µs, while DORT2002 with two channels takes around 4ms for the same result, i.e. Kubelka-Munk is about 100 times faster. However, using DORT2002 with twenty channels to obtain correct results takes around 5ms, while Kubelka-Munk *cannot* deliver correct results.

DORT2002 should therefore not be used with two channels for perfectly diffuse conditions. It gives identical results to Kubelka-Munk, but is much slower. For perfectly diffuse conditions DORT2002 should be used with, say, twenty channels for correct answers, or Kubelka-Munk should be used if its level of accuracy is acceptable. For non-diffuse conditions DORT2002 is the only alternative for correct results.

A comment should also be made on the user-friendliness of the models. As mentioned above, the explicit form and ease of use of the Kubelka-Munk equations are probably reasons for their widespread use, and they can be handled by almost anyone. Still, users need to know some mathematics to use them, and often need to create their own small computer program or spreadsheet. The equations behind DORT2002 are necessarily much more complicated. Therefore DORT2002 has been given a graphical user interface to make the calculations convenient and accessible. It works like a shell that encapsulates the parameters and the function calls. This makes it possible for any applied user to handle DORT2002. They are then free to concentrate on the application without bothering about mathematics or programming. It is also possible to call DORT2002 from a command prompt, which may be preferred by the experienced user, or to embed DORT2002 as a component in a script or a larger application. Other possibilities include building DORT2002 into applications such as automated process and quality control.

7. Future Work

Papers I and II mention two opportunities to increase the speed of DORT2002. One concerns faster ways of evaluation of the normalized associated Legendre functions, Λ_l^m, for indices l and m from 1 to fairly large numbers. The other concerns generation of sparse matrices in MATLAB. Due to the internal representation of the sparse data structure in MATLAB, it is sometimes an unsatisfactorily time consuming task to build a sparse matrix even if the non-zero elements and their row and column indices are known. Paper II also suggests investigating somewhat more elaborate convergence criteria for making earlier termination of loops more efficient.

As mentioned in Papers I and III, an upcoming research activity will be the inverse problem for DORT2002. This includes the study and development of fast and numerically stable algorithms for parameter estimation. The parameter estimation will be carried out to fit model simulations to angle-resolved light scattering measurements or to desired angle-resolved light scattering patterns. This opens the possibility of indirectly measuring parameters that are hard to determine in other ways, but also of constructing materials with designed optical properties. The starting point is known intensities in different directions, in the form of measurements or design goals, and known boundary conditions. The need for this is made clear in Paper III, where it is noted that if Kubelka-Munk is used to determine s and k values for a sample where the effect of finite thickness is large, the s and k values will also contain these errors, which will be carried over to a more accurate model if it uses these s and k values. This means that the more accurate model needs to have its own solution procedure to determine its scattering and absorption parameters. While, as discussed earlier, the Kubelka-Munk equations are easily invertible, for many models the problem of identifying parameters is not straightforward, and in many cases it amounts to an inverse problem. A solution method for the problem of determining parameters of DORT2002 is under development. In addition to this, it will be necessary to deal with the problem of surface effects, such as gloss, in real-life measurements.

To establish the implications of the effect of finite medium thickness for the application of the Kubelka-Munk model, further investigation is needed, as suggested in Paper III.

As mentioned earlier in this thesis, DORT2002 is prepared to be combined with a surface model to handle gloss. It would be interesting to evaluate such a combination, and any suggestions for a suitable surface model are most welcome. DORT2002 is also prepared for a future implementation of fluorescence to handle the effect of OBA (optical brightening agents). A proper model for the intensity transfer between wavelengths in the fluorescence process is then needed for the relevant materials. A method to handle layers with different indices of refraction has been described [20], and can readily be included in DORT2002 if desired. This includes refraction and total reflection at the boundaries, described by Snell's law and Fresnel's formulas. This would give an exact model of what is approximated by the Saunderson [21] correction in the Kubelka-Munk case.

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