Mathematical Modelling of Light Scattering in Paper and Print

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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.