

A grid approach to optimizing color recipes

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Abstract

We show that the accuracy of predicting color recipes for solid colors using the conventional Kubelka-Munk model can be improved by using grid-based empirical techniques.

We first identify the regions in color space where such improvements would be most useful. These turn out to be the dark red, dark blue and the off-white regions. In these regions of color space, we create grids using several different methods: Delaunay triangulation and Adaptive meshing techniques with thresholds either on non-linearity or on fixed distances between grid points. This last method was shown to work best for this application.

In order to match an arbitrary point in color space, based on the created grid, two different interpolation methods were tested: Linear optimization (where a linear relation between concentration space and color space is assumed within each grid cell) and Local K and S determination (where values of the Kubelka-Munk parameters are allowed to vary over color space). Our results show that grid methods using Local K and S determination lead to a significant improvement in accuracy as compared to conventional Kubelka-Munk methods.

Introduction

For solid colors, the optical model developed by Kubelka and Munk [1][2][3] and completed by the well-known Duncan rule [4] and Saunderson correction [5], is known to generally provide reasonably accurate predictions of reflectance spectra for any colorant mixture. However, for imitating a color by mixing a set of known colorants the inverse process is needed. Although calculating a color recipe based on a measured reflectance spectrum is not analytically solvable, in the paint industry this problem is routinely solved with numerical methods [6][7][8].

When the color recipes thus found are sprayed out and the corresponding reflection spectra are measured, errors still remain. These errors may originate from imperfections in the Kubelka-Munk model, from physical or chemical interactions not accounted for in the Duncan rule and/or Saunderson correction, from characteristics in the application process or from other causes yet unknown.

In order to improve accuracy, more sophisticated optical models have been developed, e.g. those based on multiframe theory [9,10]. But in spite of the steep increase in physical, mathematical and numerical complexity of these models as compared to the Kubelka-Munk approach, so far the new models did not lead to significant improvements in predicting reflection spectra for solid colors based on actual paints.

Instead of trying to derive a more accurate optical theory as a way to improve the calculation of color recipes, we have developed a more practical approach. In this approach, we design a grid in color space. This grid design is optimized by requiring that it needs to cover the required part of color space with a minimum amount of grid points. But we also require that

every point in color space should be sufficiently close to the neighboring grid points to enable interpolation of the corresponding colorant concentrations. In this way we aim at eliminating all errors due to the optical models and/or the application process.

We have organized this article as follows. We first provide a short overview of previous colorimetric work on grid methods. In section 3, we locate the regions in color space where current methods have the worst performance. For these regions, we investigate the best way to generate a colorimetric grid (section 4). In the following sections, we introduce different interpolation methods, and give details on the experimental test. In section 7, our results identify which interpolation method works best for this particular application, and we discuss the implications of this work for the color formulation process.

2 Previous work on colorimetric grids

Partitioning of color space is a technique that has been proposed for several other applications. For example, Menegaz *et al.* used Delaunay triangulation to derive a computational model for color naming [11].

To enable the calculation of color recipes, grid based approaches roughly similar to those described here have been proposed for characterizing printers [12][13][14]. These approaches are often based on rectangular cells such as in the cellular Neugebauer model [15][16], but grids based on tetrahedrons similar to the ones described here have been developed for printer characterization as well [17]. One of the alternative approaches that we consider is Delaunay triangulation. This method has been used in the past to calculate the color gamut for different media, including halftone printing [18].

3 Finding the most relevant color regions

The new approach is meant to be an improvement over the current method, in which the calculation of color recipes is mainly based on the optical model (Kubelka-Munk theory, together with Duncan rule and Saunderson correction). Therefore, the most relevant color regions for this investigation are the regions where the current method performs worst.

We therefore selected 100 clusters in CIE-Lab color space. From our color formulation databases, we selected 14.260 colors for which color recipes were available in three different paint products (waterborne and solvent borne basecoat-clearcoat systems, and high-solid topcoat). Reflection measurements on the spray outs for these color recipes were compared with the reflection spectra predicted by the optical model. The color differences between these spectra were used as an indicator for the accuracy of the optical model.

We found that in three regions of color space, the optical models showed less accuracy than in the rest of color space. These regions showed the largest percentage of colors with a model error $dE_{\text{cmc}}(1.5:1) > 0.8$. The color coordinates for these regions are shown in Table 1. In this article, we will denote

these regions as dark red, dark blue and off-white. We developed and tested our techniques in these three regions, since their accuracy in the rest of color space is expected to be better.

Table 1 Most relevant color regions

Color region	L*	a*	b*
Dark red	+13.3 to +19.5	+4.5 to +8.1	-3.5 to +2.3
Dark blue	+12.5 to +16.0	-1.5 to +1.1	-10.1 to -7.8
Off-white	+86.1 to +96.0	-4.4 to +3.4	-3.2 to +12.6

4 Creation of the colorimetric grid

We will discuss several techniques that are available for creating a grid in CIE-Lab color space. Once a grid is chosen, any position in color space is enclosed by four grid points. Thus, cells are formed by sets of four grid points. Within each cell, only four colorants (black, white and two additional colorants) are needed to cover the corresponding volume in color space. If adjacent cells utilize the same set of four colorants, they are grouped together in sub-grids. However, we found that it was not possible to formulate any of the color regions identified in the previous section by utilizing only one single set of four colorants. Therefore, each of the color regions is subdivided into several sub-grids. We note that this analysis is based on D65 illumination only. Adding more light sources

is possible, but this would increase the dimensionality and hence also the complexity of the problem.

A straightforward approach to create a grid in CIE-Lab space is to place grid points on a regular lattice with fixed mutual distances. Based on the most efficient way to pack spheres, a face centered cubic lattice was investigated. From the grid points, cells were constructed by using the well-known method of Delaunay tessellation [19][20]. This method is illustrated for the two dimensional case in Figure 1. First, non-overlapping triangles are determined that fill the convex hull of the grid points, in such a way that edges are shared by at most two triangles. The efficiency of the grid points is ensured by demanding that the encompassing circle for each triangle contains no other grid points [21].

As an alternative method for grid creation, we investigated the adaptive meshing technique proposed by Krivánek *et al.* [22]. In our implementation of this technique, the distance between grid points varies over color space, depending on the non-linearity of color coordinates as a function of colorant concentrations. This non-linearity is estimated from calculations with the optical model. We note that in this way, we do not assume that the optical model gives accurate color predictions for any given colorant mixture, as is assumed in standard approaches. Instead, we only assume that the optical model is able to indicate the relative degree of non-linearity for different parts of colorspace.

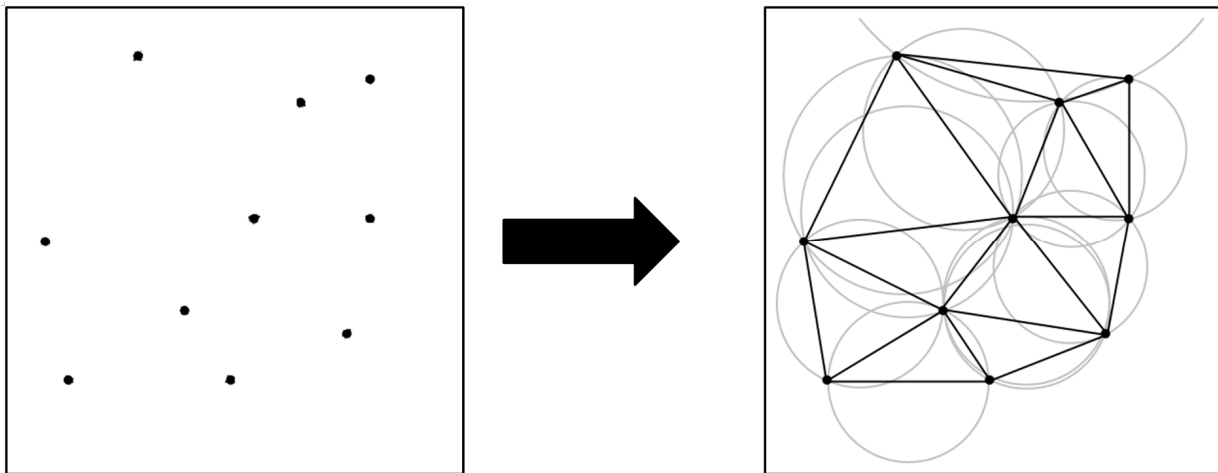


Figure 1. Grid points are connected in CIE-Lab space by using Delaunay tessellation.

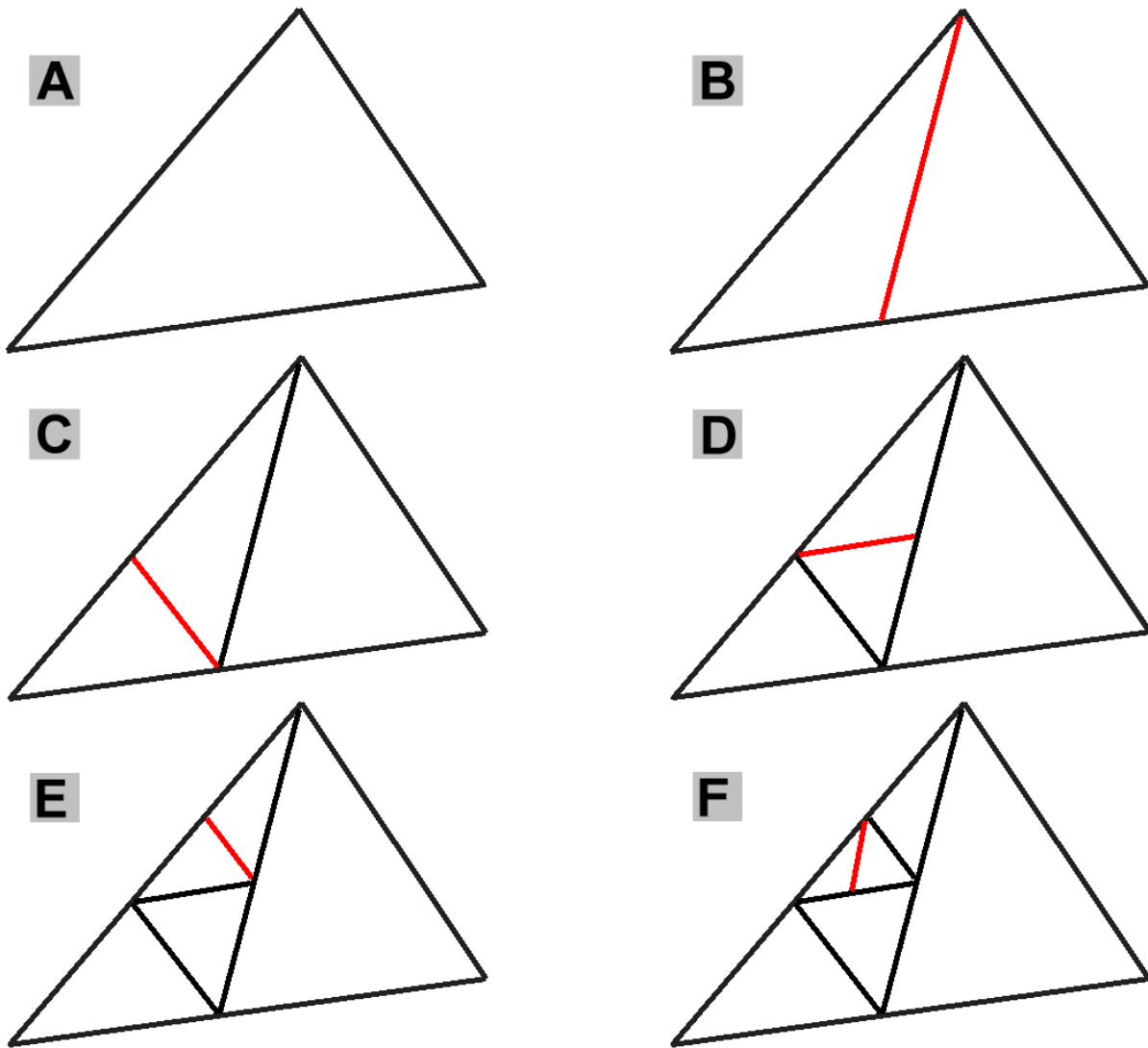


Figure 2. Adaptive meshing technique for creating a grid in color space. For reasons of clarity, the process is shown here in 2D space.

In our implementation, we investigate the reflection curves predicted by the optical model along each of the six sides of the tetrahedron formed by a set of four neighboring grid points. The degree of non-linearity along each of the six sides is calculated, and the side with the largest predicted non-linearity is identified. A new grid point is then created along this side, at the place where non-linearity is largest. This also creates new tetrahedrons, and the process is repeated for the new tetrahedrons as well (Figure 2). In an iterative process this leads to grid points for which all sides of the corresponding tetrahedrons have a degree of non-linearity below a specified threshold value.

We also tested the performance of a technique in which the adaptive meshing technique was based not on a specified threshold in non-linearity, but on a specified distance between grid points.

5 Interpolation methods

One basic assumption of our approach is that grid points are sufficiently close to each other that we can assume that a good color recipe for any point in color space is found by a linear interpolation of the color recipes corresponding to the four grid points surrounding it (otherwise, more advanced

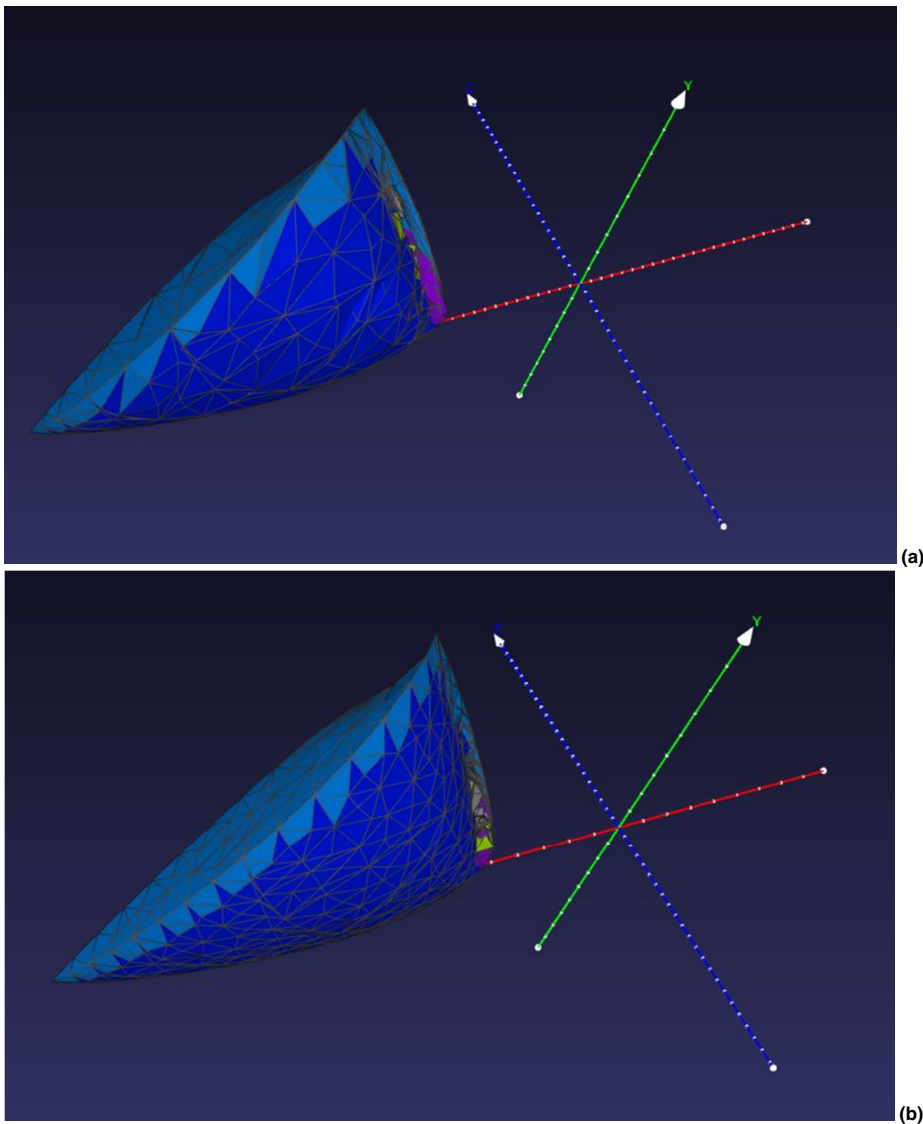


Figure 3. Grid created with adaptive concentration method using (a) a fixed theoretical interpolation error, and (b) fixed distances in color space.

interpolation methods need to be used, such as those proposed for draw down formulation in Ref. [23]). The most straightforward method for linear interpolation is to assume that this linear relation holds between colorant concentration space and CIE-Lab color space, or any other standard color space. This assumption is valid if grid points are close enough. Our results showed that the accuracy could be slightly improved if we used a color space based on CIE- L^* and the chromaticity coordinates x and y . We will refer to this method as linear interpolation.

We carried out some initial tests with linear interpolation using six pairs of samples separated by typically $dE_{ab} = 10$. These tests indicated that increasingly fine grids, with distances between points decreasing from $dE_{ab} = 10$ to 1, lead to average interpolation errors decreasing from $dE_{ab} = 0.2$ to 0.06 (see Figure 4). Obviously, a balance needed to be found between minimizing the interpolation error without needing to spray too many grid points.

We also tested an alternative interpolation technique, that we have called local K and S determination. In this method, local adjustments to the Kubelka-Munk K and S parameters are made to improve the accuracy of the optical model. In this approach, we assume that the values of the K and S parameters for all colorants have been calculated with conventional methods, based on well-chosen mixtures and covering a major part of color space [24].

Since the resulting K and S values are supposed to be valid for the entire color space, they are referred to as the global K and S values. In order to derive locally adjusted values for the K and S parameters, we used the following approach. For a given point in color space, the four grid points of the enclosing tetrahedron are identified. For the colorant mixture corresponding to each of these four grid points, the global K and S values are calculated based on the global K and S values of the constituent colorants. However, for each of the grid points, reflection measurements of the

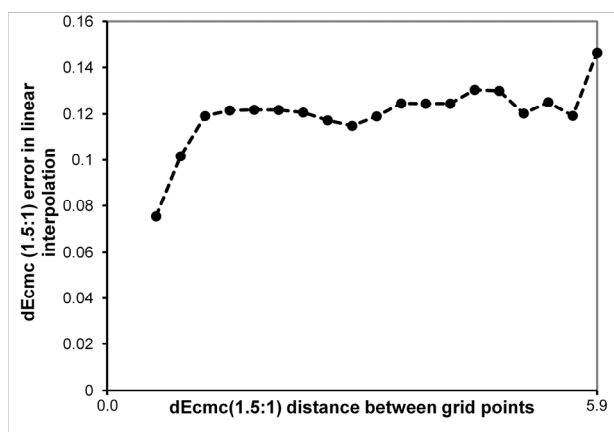


Figure 4. Model errors due to linear interpolation, as a function of the distance between grid points in color space.

sample are available. Using the standard Kubelka-Munk equation, these measured reflection values are converted to the ratio between the so-called local K and S values. We adjust the global K value for the mixture corresponding to a grid point by a multiplicative factor f , in such a way that the local K value is exactly reproduced.

Note that the dependence on wavelength of K, S and f parameters is accounted for throughout the analysis, but suppressed in the notation.

We also note that in those cases in which more than one combination of colorants is able to enclose a certain part of color space, we chose the optimal combination of colorants based on a metric that combines colorimetric properties, price and application properties.

6 Experimental

For this test, we selected 50 target colors that are actual car paints, and for which we want to test the accuracy of predicting color recipes. Based on our identification of the color regions most relevant for this investigation, we selected 20 dark red colors, 20 off-white colors and 10 dark blue colors.

We have tested two different methods for calculating color recipes: Linear interpolation, and Local K and S determination. As a reference, we used the conventional method of calculating color recipes with Kubelka-Munk. Therefore, color recipes for the 50 target colors were calculated with 3 methods, resulting in 150 paint samples.

Further, a total of 498 grid points were created, the corresponding color recipes were sprayed out and the reflection spectra of the resulting samples were measured. Actually, for 256 grid points this process was repeated in order to test reproducibility of the method. In order to formulate the selected 50 target colors, we found that we needed 14 different colorants. The global K and S values of these colorants were estimated based on a total of 142 different mixtures.

Therefore, a total of 1046 color formulas were designed and sprayed out, and the corresponding reflectance spectra were measured. The processes of mixing colorants, paint application and reflection measurement were fully automated in order to eliminate human errors.

For the reflection measurements we used the BYK-Mac instrument. The multi-angle measurements were converted to effective $d/8$, gloss-included measurements by using a linear regression technique developed by Berns and Petersen [25].

7 Results and discussion

When creating the grid, we found that the method of Delaunay tessellation works fine as long as colors are taken that are remote from the boundary of the color solid. However, problems arise for colors close to that boundary, in the regions where the color solid is concave. Delaunay triangulation is problematic for describing the boundary of the color solid, since it is not a convex hull in CIE-Lab space. With Delaunay triangulation, concavities in the color solid are filled, resulting in cells lying outside the color solid. Obviously during interpolation this leads to attempts to match colors lying outside the color solid, which is not possible. In the literature, methods have been proposed for the Delaunay triangulation of concave volumes, but no complete solution has been found yet.

The adaptive mesh techniques do not have this problem. Grids created by this technique nicely follow the shape of the color solid. Further, the method distributes the error due to interpolation uniformly over color space, by subdividing it further in those areas where the relation between concentration space and color space is most nonlinear [22]. However, when we used the adaptive mesh technique as based on non-linearity thresholds, we encountered a different problem. The resulting grid cells became very irregularly shaped (Figure 3a). This is caused by the strongly anisotropic character of the non-linearity in color space. Only by basing the adaptive mesh technique on fixed distances in color space, this problem was avoided (Figure 3b). For this reason, this technique was used in our evaluation of the grid approach to predicting color recipes.

As mentioned before, we have tested three different methods to predict color recipes: the conventional Kubelka-Munk method, Linear interpolation and Local K and S determination. For each of the 50 target colors the three resulting color recipes were sprayed out, and the reflection spectra of the samples were measured. We calculated the color difference between the sample and the target color. The results are shown in Table 2.

Table 2 Accuracy of different methods to predict color recipes.

Method	Color difference $dE_{CMC}(1.5:1)$		
	Average	Min.	Max.
Conventional Kubelka-Munk	0.67	0.20	1.86
Linear interpolation	0.68	0.09	2.35
Local K and S determination	0.37	0.09	0.71

Based on the results shown in Table 2, it can be concluded that the method using local K and S values is the most accurate. The results are considerably better than those obtained when using the Conventional optical model (Kubelka-Munk) or Linear interpolation. It is also more consistent than the other two methods, in the sense that it avoids cases with large errors.

Generally, our results show that the method using Local K and S determination can be expected to work very well, since

in many cases the resulting color accuracy is better than what is required for a visual approval.

For this reason, the grid-based techniques developed in this investigation are recommended as a method to improve the accuracy of predicting color recipes.

In future work, we plan to explore similar techniques for higher dimensional systems, by extending this work to color matching under several different illuminants, and to effect coatings that need to be matched under several different measurement geometries. We will also investigate a method to solve problems that occur when color formulas are not completely hiding. These problems generally can be avoided by using a suitably colored substrate, but in the grid approach there will be neighboring cells that use differently colored substrates. Since the color difference between substrates used for adjacent cells are expected to be small, we will investigate the color accuracy in case all substrates are assumed to be of the same color.

References

- [1] P. Kubelka and F. Munk, "Ein Beitrag zur Optik der Farbanstriche". Zeitschrift für Technische Physik, 11a, 593-601 (1931).
- [2] P. Kubelka, "New contributions to the optics of intensely light-scattering materials. Part I." J. Opt. Soc. Am., 38, 448-457 and 1067 (1948).
- [3] P. Kubelka, "New contributions to the optics of intensely light-scattering materials. Part II: Nonhomogeneous layers". J. Opt. Soc. Am., 44, 330-335 (1954).
- [4] D.R. Duncan, "The colour of pigment mixtures". Proc. Phys. Soc. London, 52, 390-400 (1940).
- [5] J.L. Saunderson, "Calculation of the color of pigmented plastics". J. Opt. Soc. Am, 32, 727-736 (1942).
- [6] P. Koirala, M. Hauta-Kasari, B. Martinkauppi and J. Hiltunen, "Color mixing and color separation of pigments". Color Res. Appl., 33, 461-469 (2008).
- [7] K. Unterforsthuber, Theoretische Grundlagen der Farbrezeptberechnung (Unterforsthuber, Frankfurt, 2005).
- [8] G.A. Klein, Industrial Color Physics (Springer, New York, 2010).
- [9] P.S. Mudgett and L.W. Richards, "Multiple Scattering Calculations for Technology". Appl. Opt., 10, 1485-1502 (1971).
- [10] P.E. Pierce and R.T. Marcus, "Radiative Transfer Theory solid color matching calculations". Color Res. App., 22, 72-87 (1997).
- [11] G. Menegaz, A. Le Troter, J. Sequiera and J.M. Boi, "A discrete model for color naming". Eurasip J. Appl. Signal Process, 2007(1), 113-129 (2007).
- [12] S.M. Chosson and R.D. Hersch, "Visually-based color space tetrahedralizations for printing with custom inks", Proc. SPIE, vol. 4300, pg. 81-92 (2001).
- [13] H. Boll and S. Gregory, "Color-to-ink transformation for extra-quarternary printing". US patent 5563724 (1994).
- [14] H. Boll, "N-colorant gamut construction". US patent 7411701B2 (2004).
- [15] J. Morovic, P. Morovic, M.G. Encrenaz, J. Lammens and Y. Richard, US patent 2010/0214576 (2010).
- [16] D.R. Wyble and R.S. Berns, "A critical review of spectral models applied to binary color printing". Color Res. Appl., 25, 4-19 (2000).
- [17] J.Y. Hardeberg, Acquisition and reproduction of color images. PhD thesis (Ecole Nationale Supérieure des Telecommunications, Paris, 1999).
- [18] X. Zhao, "Generic device color gamut description". Color Res. Appl., 32, 394-408 (2007).
- [19] J. F. Thompson, B.K. Soni, N.P. Weatherill, Handbook of grid generation (CRC Press Boca Raton, London, 1999).
- [20] B. Delaunay, "Sur la sphère vide". Bull. Acad. Sci. USSR(VII), 793-800 (1934) Classe Sci. Mat. Nat.
- [21] P.O. Persson and G. Strang, "A simple mesh generator in MATLAB". SIAM Rev. 46, 329-345 (2004).
- [22] J. Krivánek, S. Pattanaik and J. Zara, "Adaptive mesh subdivision for precomputed radiance transfer", Proc. 20th Spring Conference on Computer Graphics SCCG'04, Bratislava, pg. 104-109 (2004).
- [23] C. Vignolo, "Farbtonanpassung unter Verwendung eines alternative Verfahrens zur Bestimmung der Wirkungsmatrix von Pigmenten in Lacken". German Patent DE 10 2008 052 300 A1 (2008).
- [24] J.H. Nobbs, "Colour-match prediction for pigmented materials". Chapter 6 in: R.McDonald, ed., Colour Physics for Industry, (Society of Dyers and Colorists, Bradford, 1997) pg. 292-372.
- [25] R.S. Berns and K.H. Petersen, "Empirical modeling of systematic spectrophotometric errors". Color Res. Appl., 13, 243-256 (1988).

Author biography

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