The thesis explores prospects and application areas concerning the use of spectral imaging to solve various problems. In practice, spectral properties of a scene can be used for scene understanding, object recognition or material identification. The challenge is in developing computational methods to extract and analyze the physical properties encoded in the reflectance. This thesis contributes in that track addressing problems that are needed to be solved especially in cultural heritage.
G M ATIQUR RAHAMAN

Use of Reflectance Measurements to Study Turbid Media by Imaging

Publications of the University of Eastern Finland
Dissertations in Forestry and Natural Sciences
No 263

Academic Dissertation
To be presented by permission of the Faculty of Science and Forestry for public examination in the Louhela Auditorium in Joensuu Science Park at the University of Eastern Finland, Joensuu, on March, 27, 2017, at 12 o’clock noon.

School of Computing
ABSTRACT

Optical measurements by imaging represent a non-destructive form of technology that can be used to solve varied problems in many application areas, particularly, in cultural heritage. The state of art spectral imaging offers great potential to extract and analyze the physical properties of objects in novel ways using spectral reflectance information beyond the visible range and at high resolutions. This thesis focuses on imaging techniques to address several problems relevant to color reproduction and analysis of colorant in turbid media. The first part of the thesis addresses a fundamental issue (light/ink/paper interactions) in developing spectral color printing technique. The second part deals with methods for analyzing the colorants of textile objects.

In the first part, so as to better understand the light/ink/paper interactions and their effect on the color reproduction model, a set of microscale images of halftone prints was analyzed. The k-means clustering algorithm segmented the print area into solid ink, unprinted paper, and an ink-paper mixed area. The results were then used to characterize the dot gain, a phenomenon that challenges the accuracy of color prediction models. Based on the image analysis, an expansion of the classic Murray-Davies (MD) reflection formula was proposed for halftone printing. In addition to demonstrating an improved prediction accuracy, the proposed model provides a better explanation of the media interactions.

To enhance our understanding of the aforementioned issue, a spectral camera was employed to examine the microstructure of the halftone images in detail. The existing models were investigated to characterize the changes in the micro-color of the paper and ink. A hierarchical cluster analysis was applied for the image segmentation and thus to determine the model parameters. After accounting for the effect of the solid ink and mixed area, a more precise explanation was obtained regarding the single-model parameter that manifests the light scattering effect. A series of halftone patches printed with various properties was
analyzed, and the results supported the proposed expansion of MD formula.

In the second part, the wavelength regions of reflectance spectra of dyed fibers were investigated in order to classify the dyes as either natural or synthetic. As samples, dyed fibers of wools with a wide range of physical and optical color properties were measured using a spectral line scan camera in the wavelength range of 400–2500 nm. A small number of highly discriminating bands in the 1000–2500 nm range were explored for the effective spectral classification of the fiber dyes. A logistic regression-based feature selection algorithm determined the bands, and the support vector machine classifier with a polynomial kernel yielded over 97% accuracy.

To detect the spectral color discrepancies of fibrous surface, images of traditional carpets and kilims were visualized in the range of 400–1000 nm. The visualization of the surface through the red, green and blue (RGB) values rendered by the extended CIE (International Commission of Illumination) color matching functions was the most effective in revealing and interpreting the tone variations. The visual inspections of the rendered images readily identified the spectral color variations that were either invisible or low-contrast in reality. Moreover, the objective metrics showed a substantially higher contrast between the normal and degraded color regions with respect to the conventional RGB image.

*Universal Decimal Classification: 535.33, 535.6, 620.179, 667.622, 681.7, 904*

*Library of Congress Subject Headings: Nondestructive testing; Optical measurements; Spectral imaging; Image analysis; Imaging systems; Reflectance; Spectral reflectance; Color; Colorimetry; Wavelengths; Hierarchical clustering (Cluster analysis); Color printing; Dyes and dyeing; Textile fibers; Wool; Cultural property*

*Yleinen suomalainen asiasanasto: rikkomaton aineenkoetus; optiset ominaisuudet; kuvantaminen; spektrit; spektrikuvaus; heijastuminen; väri; aallonpituuus; väripainatus; väriaineet; luonnonkuidut; villa; kulttuuriperintö*
Preface

Bismillahir Rahmanir Rahim

The research for this study was carried out in the company Voxvil AB and Digital Printing Center, Department of Natural Science at Mid Sweden University during 2012-2014 and in the School of Computing at the University of Eastern Finland during 2015-2017. Parts of this study was supported by the EU Marie Curie Initial Training Networks (N-290154, CP7.0), and the Information and Communication Technology (ICT) Division of Bangladesh. The supports are gratefully acknowledged.

First, I express my gratitude to almighty Allah the most gracious and the most merciful for his support. Then I express my gratitude to my supervisors Prof. Jussi Parkkinen and Prof. Markku Hauta-Kasari for accepting me as a PhD student and their continuous support during my study. I thank Dr. Ole Norberg and Prof. Per Edström for their supervision during the study of Licentiate degree in Mid Sweden University. I also remember all the colleagues in CP7.0 project that gave me a large opportunity to be introduced and work in the industries.

I want to thank to the department staff and all members (past and present) of the color research group in Joensuu with whom I have worked since my CIMET master study in 2010-2011. Especially, Dr. Ville Heikkinen, and Dr. Pauli Fält for important discussions on different aspects of spectral methods.

I thank my son Arian Rahman and daughter Tasnim Rahman for their incredible endurance during my stay at abroad. During this period, my wife Habina Nasrin’s amazing care of our children was remarkable.

Joensuu, March 2017

G M Atiqur Rahaman
## NOTATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu )</td>
<td>frequency</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>wavelength</td>
</tr>
<tr>
<td>( s )</td>
<td>light scattering coefficient</td>
</tr>
<tr>
<td>( \beta )</td>
<td>surface roughness</td>
</tr>
<tr>
<td>( \theta_i )</td>
<td>angle of incidence</td>
</tr>
<tr>
<td>( k )</td>
<td>light absorption coefficient</td>
</tr>
<tr>
<td>( L_r )</td>
<td>intensity of the reflected light</td>
</tr>
<tr>
<td>( L_i )</td>
<td>intensity of the incident light</td>
</tr>
<tr>
<td>( R_0 )</td>
<td>reflectance of bare paper with black background</td>
</tr>
<tr>
<td>( R_g )</td>
<td>reflectance of bare paper with a background</td>
</tr>
<tr>
<td>( R_a )</td>
<td>reflectance of an opaque pad</td>
</tr>
<tr>
<td>( \tau )</td>
<td>transmittance</td>
</tr>
<tr>
<td>( \theta )</td>
<td>polar angle</td>
</tr>
<tr>
<td>( \phi )</td>
<td>azimuth angle</td>
</tr>
<tr>
<td>( \phi )</td>
<td>spectral radiant flux</td>
</tr>
<tr>
<td>( E )</td>
<td>spectral irradiance</td>
</tr>
<tr>
<td>( L )</td>
<td>spectral radiance</td>
</tr>
<tr>
<td>( \tau_f )</td>
<td>reflectance factors</td>
</tr>
<tr>
<td>( L )</td>
<td>spectral power distribution (SPD) of light</td>
</tr>
<tr>
<td>( R )</td>
<td>reflectance factor</td>
</tr>
<tr>
<td>( d )</td>
<td>signal detected at the sensor</td>
</tr>
<tr>
<td>( C )</td>
<td>spectral sensitivity of the sensor</td>
</tr>
<tr>
<td>( \eta )</td>
<td>dark noise of the sensor</td>
</tr>
<tr>
<td>( l )</td>
<td>vector of SPD of L</td>
</tr>
<tr>
<td>( r )</td>
<td>vector of reflectance factors</td>
</tr>
<tr>
<td>( c )</td>
<td>vector of sensor sensitivity</td>
</tr>
<tr>
<td>( w )</td>
<td>vector of joint effect of light and sensor’s sensitivity</td>
</tr>
<tr>
<td>( W )</td>
<td>matrix having ( w ) as the columns</td>
</tr>
<tr>
<td>( d )</td>
<td>vector of signals detected at the sensor</td>
</tr>
<tr>
<td>( A )</td>
<td>absorbance</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>the length of light path</td>
</tr>
<tr>
<td>( \Omega )</td>
<td>closed range of wavelengths</td>
</tr>
<tr>
<td>( I )</td>
<td>represents a gray level image</td>
</tr>
</tbody>
</table>
\( a_{\text{eff}} \) effective or actual coverage of ink in halftone print
\( a \) reference/nominal coverage of ink
\( a_t \) coverage of solid ink
\( a_{\text{mix}} \) coverage of mixed ink/paper area
\( a_P \) coverage of unprinted paper area
\( a_{\text{solid}} \) fractional coverage of solid ink area
\( a_{\text{tot}} \) total dot gain
\( \hat{r} \) vector of predicted reflectance
\( \text{sRMS} \) spectral root mean squared error
\( n\)-factor Yule-Nielsen (YN) n factor
\( lpi \) lines per inch
\( dpi \) dots per inch
\( T_{\text{paper}} \) tristimulus value (TSV) of white (unprinted) paper
\( T_{\text{pap}} \) TSV of paper between ink dots in a halftone print
\( T_{\text{limit}} \) TSV of paper when ink coverage is just below 100%
\( T_{\text{ink}} \) TSV of full-tone (100%) ink in a halftone print
\( T_{\text{dot}} \) TSV of dots of arbitrary ink coverage
\( T_{\text{halftone}} \) overall TSV of a halftone print
\( \bar{r}, \bar{g}, \bar{b} \) CIE RGB color matching functions
\( \bar{x}, \bar{y}, \bar{z} \) CIE XYZ color matching functions
\( X, Y, Z \) coordinates in CIE XYZ color space
\( R, G, B \) coordinates in CIE RGB color space
\( V_\lambda \) luminous efficiency curve
\( x, y \) coordinates in CIE (x,y)-chromaticity diagram
\( I \) image vector
\( \mu \) mean of a set of value
\( d \) calculated distance between two points
\( x_i \) i-th measurement vector of reflectance
\( y_i \) class label for \( x_i \)
\( X \) training data containing \( x_i \) and \( y_i \)
\( \mathcal{R} \) the real numbers
\( \alpha \) coefficient in a model
\( \alpha \) vector of \( \alpha \)
\( \tau_{\lambda,1} \) spectral transmittance of full-tone or sold ink
\( T_{\text{solid}} \) TSV value of solid ink of arbitrary coverage
\( T_{\text{mix}} \) TSV value of mixed area of arbitrary coverage
\( p \) exponential parameter to account light scattering
\( \gamma \) regularization parameter
\( \phi \) objective function
\( \forall_i \) in the i-th space
\( r_b, g_b, b_b \) basis vectors for red, green blue color rendering
MIA microscopic image analysis
AM amplitude modulation
FM frequency modulation
VIS visible
NIR near infrared
SWIR Short wave infrared
LIST OF PUBLICATIONS

This thesis is based on following publications:


Throughout the thesis, these publications are referred to as [Paper I], [Paper II], [Paper III], and [Paper IV]. The above publications have been included at the end of this thesis having their copyright holders’ permission.
AUTHOR’S CONTRIBUTION

The publications selected for inclusion in this thesis are original research papers concerning color printer characterization, dye classification, and color defect detection of works of arts on fibrous supports.

In Paper I, the idea of using a microscopic imaging system was proposed by the co-authors. The samples were prepared by the author and printed by a professional printing company in Sweden. Dr. Daniel Nyström supplied the set of offset samples measured using a specialized microscopic RGB-spectral camera at Linköping University. The other microscopic images were made by the author with the assistance of professionals from a commercial pulp and paper research company (MoRE, Sweden). The original idea behind the image analysis and the proposed extension of a reflectance model was the author’s. The author conducted all the data analyses and numerical computations.

In Paper II, the idea of modeling the reflectance variations using spectral imaging was proposed by the author. The spectral imaging was performed by the author with the assistance of Dr. Jouni Hiltunen at the University of Eastern Finland (UEF). All the data analyses and numerical computations were conducted by the author.

In Papers III and IV, the imaging was performed by the author with the help of Dr. Laura Fauch and Dr. Dmitry Semenov. For Paper III, the textile samples were collected by the co-authors. The original idea, the data analyses, and the numerical computations were all the responsibility of the author. The author had fruitful discussions in this regard with Dr. Ville Heikkinen and Dr. Markku Keinänen. For Paper IV, the carpets were collected by the co-authors. The original idea of defect detection by extending the RGB color was the author’s. The author conducted all the data analyses and numerical computations.

The author has written the manuscripts for each of the included papers. The reviews provided by the co-authors were helpful.
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1 Introduction

Fibrous supported artworks such as paintings and, historical textiles like carpets, clothes, tapestries, shrouds etc. are all objects of great cultural, art and historic (A&H) significance [1, 2, 3]. Color is among the most common and significant aspects as colorants have been used in these A&H objects since prehistoric times. Dyes represent the main colorants that have been used either directly or in forms such as pigments [2]. The scientific study of the different color aspects of such objects yields knowledge and various insights regarding technology and traditions, which might be impossible to obtain through alternative means [4, 5, 6].

Unfortunately, the colorants and fiber supports both are prone to deterioration through various mechanisms, resulting in a change in the overall color, fading, and stains. There are different types of photochemical processes that lead to color degradation and colorant deformation [7]. Moreover, as age increases, the objects become increasingly fragile, thereby becoming candidates for further deterioration or damage through handling, non-standard storage, or poor restoration [8]. Therefore, the unique A&H objects need to be restored and protected against such damage. At the same time, since some of the reasons for the deterioration are natural or unavoidable, digital reproduction is necessary for true, precise, and complete documentation [9, 10, 11, 12].

Among other functionalities of digital reproduction, the reliable color printing of artworks is essential from various perspectives in the context of museums and art galleries [13]. For example, accurate color printings can be used for display, analysis, or to plan restoration tasks [13, 14, 15]. Since conventional colorimetric printing has inherent technological limitations, multichannel or spectral printing is required for the true and precise color printing of artworks [10, 13, 16, 17, 18, 19]. However, multi-disciplinary problems are required to address in
order to develop multi-channel or spectral printing technology [20]. In this regard, part of this thesis work is relevant to modelling the light/ink/paper interactions necessary for the characterization and calibration of the printers. The work was accomplished by participating in a project (cp70.org) intended to develop new technology for spectral print reproduction [20].

In terms of art restoration technology, most of the methods available for colorant analysis require samples to be removed from the A&H objects, followed by a non-trivial preparation method [2, 6, 21, 22, 23, 24]. Although these diagnostic technologies are very precise and accurate, conservators do not commonly prefer due to the damage they cause [10]. Instead, non-destructive, non-contact, and spatially resolved spectral techniques are more widely being adopted to analyze various aspects in the field of cultural heritage [9, 25, 26, 27, 28, 29]. Improved tools for spectral analysis and/or visualization is thus demanding to conservators [10, 29]. Part of the thesis is about developing methods to facilitate non-destructive analysis of dyes and advanced visualization of A&H objects.

This thesis mainly focuses on imaging technique for the characterization of light/ink/paper interactions of halftone prints, analysis of dyes in textiles, and visualization of colored surfaces. Paper and textile fibers are both optical turbid media, which means light penetrates, interacts inside the media, and exits out of the surface. The overall diffuse reflectance is thus the result of light scattering and absorption [30], and contains information about the colorants and the media components. In spectral imaging, the reflectance measurements are made in a series of narrow and contiguous wavelength bands that represent useful information. Such between-band information can expand and improve the capability of object analysis on a pixel-by-pixel basis. Therefore, spectral reflectance measured by imaging technique is the key aspect considered for analyzing the relevant problems in this thesis.

Characterization of color printers

In reality, most print reproductions of paintings are poor owing to the inherent limitations of the conventional colorimetric
Introduction

printing technology that reproduces the color consistent for only one viewing condition [31, 32, 33, 34, 35]. This problem can be minimized by spectral printing that aims to reproduce the given spectral reflectance rather than the colorimetric values [14, 15]. Though multidisciplinary problems are addressed to realize this technique [20], the color prediction model (CPM) is central to the development of this technology [36]. Further, the type of paper, printer, halftoning method, and ink substantially influence the performance of color modeling, mainly due to the dot gain phenomena.

Modelling the dot gain effect on the color prediction model is a primary issue. Ink spreading, penetration, and lateral light scattering are the causes of dot gain. In fact, the accurate characterization of the light/ink/paper interactions is essential for the calibration of any printing technique. The existing characterization techniques are semi-empirical and mainly based on the classic Murray-Davies (MD) reflection model [36]. The key aspect of this procedure is optimization of the model parameters with respect to the macroscopically measured reflectance of a set of sample prints. Although this method works reasonably well, there remains a lack of understanding regarding the halftone media interactions.

Furthermore, while the monochrome MD formula is the source of many successful color models, the formula itself generates large prediction errors. The basic MD formula sets the overall reflectance as equal to the sum of the light reflected from various areas of the halftone print, thereby maintaining the law of the conservation of energy [36]. The assumption of constancy in the reflectance of ink and paper yields unacceptable errors in most cases because dot gain phenomena change the reflectance of inks and paper.

In this dissertation, microscopic views of the halftone prints were used to physically measure and analyze the model parameters that are defined as the fractional coverage of ink and paper. For the preliminary investigation, microscopic RGB imaging was used to experimentally characterize the dot gain phenomena and then correlate those phenomena to the
parameters of the color prediction models. In contrast to the conventional view, it was shown that the dot gain is better explained if the ink dots are segmented into a solid and mixed area [37]. This observation helped to suggest an extension to the basic MD reflection model in Paper I. The performance was clearly improved over the MD model, while retaining the physical plausibility of that model.

The second approach involved the microscopic spectral imaging system to measure the halftone dot patterns. The measured data were used to study and evaluate Engeldrum’s formula [38] in order to characterize the internal color changes of the ink dots and the paper between the dots. Rigorous analysis of the measured and simulated data showed that Engeldrum’s formula should be corrected. The evaluation results supported the expanded formula (proposed in Paper I) for the overall tint prediction of halftone images (as reported in Paper II).

**Colorant analysis of textiles**

Currently, the colorants of A&H textile objects are analyzed using different technologies that are very precise and accurate in detecting and identifying the chemical structures of the dye components [2, 6, 22, 23, 39]. However, most of such technologies require the removal of fibers, the extraction of the dyes, and then an analysis of the data yielded by the relevant technology [2, 6, 40]. Therefore, the initial non-destructive screening of the dyes into natural or synthetic classes [41] can save a lot of time, cost, and more importantly, part of priceless objects.

In this dissertation, the spectral reflectance of textile samples were used to classify the applied dyes into either natural or synthetic class. The spectral bands from visible (Vis) to near infrared (Vis/NIR) (400–1000 nm) and short wave infrared (SWIR) (1000–2500 nm) were investigated in order to identify the discriminative regions. A feature selection algorithm determined a small number of bands to discriminate between the dye classes. A support vector machine classifier with a polynomial kernel was used for classification. Moreover, just three bands were optimally selected and evaluated for the classification (Paper III).
Enhanced visualization of cultural objects

The colors of A&H objects can change due to natural processes that cause for the deterioration of dyes, yellowing of fibers, and development of degrading elements [7]. Moreover, careless handling, touching, or even incorrect restoration work can make damage or introduce dramatic changes in color, especially in the case of paintings [8, 42]. Therefore, studying the overall color tonality variations, detecting color defects, or even predicting potential areas likely to change color in the future is necessary when planning and applying restoration work [13, 42]. Furthermore, digitally rejuvenating the color of artworks and displaying them in an electronic display represent work commonly undertaken in museums and art galleries [17, 18].

The dyes and the natural fibers have different optical properties in (400-2500 nm) spectral range. Therefore, adding the reflectance information of the infrared region in rendering standard RGB colors should more accurately represent the physical condition of the blended fiber/dye components. In this thesis, a general approach for the enhanced visualization of colored surfaces has been investigated (Paper IV). As example objects, traditional carpets and kilims were measured on the Vis/NIR (400-1000 nm) bands in order to render them in a standard RGB display. A computational method based on stretched CIE color matching functions was used to project the spectral data on the R, G, and B channels [43, 44]. Another complementary method based on wavelength band selection for each color channel was demonstrated. The results showed that in the RGB renderings, any subtle spectral color variation is easy subject to automatic visual detection. The objective metrics of color difference justify the enhanced capability comparing the results with the standard RGB image.

The remainder of this thesis is organized as follows. First, the main aims of the thesis and how they were addressed are listed in chapter 2. Chapter 3 provides a brief description of the relevant theories, while chapter 4 describes the experimental studies and results reported in Papers I-IV. Finally, the main assertions and findings of this thesis are discussed in chapter 5.
G M Atiqur Rahaman: Use of Reflectance Measurements to Study Turbid Media by Imaging

Dissertations in Forestry and Natural Sciences No 263
2 Research Problems Addressed in the Thesis

The main aims of this thesis and the methods by which they were addressed are as follows.

1. Characterization toward a comprehensive understanding of print media (ink/paper/light) interactions and their effect on color prediction.

   ➢ A wide range of print samples as a function of paper, ink, halftoning, and printing technology were prepared. Microscopic RGB imaging was used to measure the print surface in reflectance mode. The analysis was performed following a novel strategy involving segmenting the image into solid ink, ink/paper mixed area, and unprinted paper. The dot gain measured by the image analysis was compared with the standard estimation technique. Based on image analysis results, an extension to the classic MD reflectance prediction model was proposed by adding an additional term to better account for the light. The accuracy of the proposed model was analyzed using a set of conventionally obtained parameters and the experimental image analysis. This work was published in Paper I.

2. To characterize the changes of color in the components (solid ink, mixed area and paper) of a halftone image.

   ➢ Spectral microscopic images of the same set of print samples were captured on 420 nm to 700 nm in steps of 10 nm. The characteristic behavior of the tri-stimulus values of each component was analyzed in the CIE-xy chromaticity space. Investigation was performed with the parameters of an existing model that characterizes the change of color of halftone micro
components. The performance of our proposed reflectance model was then evaluated and contrasted with that of the existing one. This work was published in Paper II.

3. Use spectral reflectance to study the colorants applied to textiles.

- Woolen yarns dyed with various natural and synthetic dyes were collected and imaged on a spectral imaging system in the range of 400–2500 nm in steps of 10 nm. Discriminative bands for the dye classification were selected using the sparse logistic regression technique and then evaluated using a support vector machine classifier. The work has been described in Paper III, which is currently under review.

4. To develop a method to automatically visualize spectral color variation of textile surface elements.

- The key principle to attain this objective was to add infrared reflectance in rendering tri-stimulus colors. Classical carpets and kilims were collected and measured using a spectral camera in the range of 400–1000 nm in steps of 10 nm. A band weighting based spectral image visualization method using stretched CIE color matching functions was applied. In addition, the band selection method using an independent component analysis (ICA) was also examined. The work has been described in Paper IV, which has been accepted for publication.
3 Theory

3.1 LIGHT-MATERIAL INTERACTIONS

Light was described by Einstein as small energy particles or photons, while Maxwell described it as electromagnetic (EM) waves that propagate at a speed of 299792 km/s. The electric and magnetic fields’ oscillations build up the EM wave motion. The frequency ($\nu$) is the number of oscillations per second, while the wavelength ($\lambda$) is the length of the wave. $\nu$ and $\lambda$ are inversely proportional because the propagation speed is constant. Fig. 3-1 illustrates the extent of EM radiation and the portion that is perceived as visible light when the $\lambda$ is between 400 nm and 740 nm [45].

![EM spectrum diagram](image)

Figure 3-1: A diagram of the EM spectrum illustrating various properties across the range of wavelengths ($\lambda$). Source: [46]

3.1.1 Effect of light on turbid medium

The refractive index, the basic optical property of a material, determines how light interacts with the material. When light illuminates any object that consists of a turbid medium (e.g., natural fibers), the surface reflects light, creating the visual appearance of the object. While part of the light is reflected from the air-surface interface (surface reflection), part penetrates into the surface. Light that has penetrated the surface may be absorbed,
scattered, and then reflected back to the surface and into the air (body reflection) [47].

As a turbid media, paper has a complex structure which usually comprises of fiber networks, fillers, colorant molecules (e.g. FWA), and air [45]. Fig. 3-2 shows a simplified paper diagram illustrating a cellulose fiber with a hollow in the middle called lumen. Reflection, refraction, scattering and transmission occur when light falls on this dielectric material and meets the fiber [48]. The light inside the surface interacts with constituting materials (e.g., lumen) and go through different events due to different optical properties. A fraction of light is absorbed and transformed into heat, whereas the remaining light is ultimately transmitted back out of the surface.

![Diagram of light-material interactions](image)

**Figure 3-2: Light-material interactions.** As the ray hits a turbid medium (e.g. the fiber), the light changes direction based on the refractive index. Fractions of light are reflected, refracted, absorbed, and transmitted.

As a result, the diffuse reflection in paper or textile products is the result of multiple reflections, refractions, and scattering or diffraction with internal particles. A bare piece of paper is perceived as a matt white surface due to diffuse reflection. Because, an almost equal amounts of lights are reflected for the entire range of visible wavelengths. Fig. 3-3 shows the light interactions in a medium that contains embedded and/or colorant particles. In this case, light is absorbed preferentially at certain wavelengths by the colorant molecules. The absorption is dominated by the chromophores that gives color appearance to the surface.
It is worth noting that scattering and absorption are ultimately manifested in diffuse reflectance. The reflectance spectrum can therefore be used to characterize materials, to identify certain groups of molecules, for example, or to identify the presence of a given substance and to estimate its quantity [45, 30]. For example, the light scattering ($s$) and absorption ($k$) coefficients are used in pulp and paper, and textile industries for optical characterization of turbid media [45].

3.1.2 Effect of surface undulations on reflectance

The distribution of reflected light on a surface depends on the direction of incident rays, and the roughness (i.e., microstructure) or topography of the surface [49]. The definition of roughness varies depending on the application area or one’s point of view. In the paper industry, surface roughness is measured as the variations in peak heights around a mean value, and is then divided into macro- and micro-roughness [45]. When the correlated length of the surface topography is of the same magnitude or smaller than the wavelength of light, roughness is referred to as micro-roughness. Otherwise, roughness is referred as macro-roughness.

Assume that the given surface is flat and the underlying material is homogeneous. If a ray of light strikes this surface, the reflected ray will lie in the same plane formed by the incident ray and the surface normal. The reflected ray will also subtend an angle with the normal equal to the angle between the incident ray and the local normal (Fig. 3-4a). This kind of reflection is referred to as specular, metallic or dielectric reflection [50]. In contrast, if
parallel rays of light strike a surface that is not perfectly flat on a microscale, the incident rays are scattered in a variety of directions (Fig. 3-4b). If the difference between the local surface normals and the average normal is small, most reflected rays will lie around the direction of ideal specular reflection. This type of surface appears glossy.

Surface roughness can also be described as a number of small facets (Fig. 3-5). If the facets are distributed with different inclinations, the surface is rough [45]. In a rough surface, the reflected light is scattered in different directions yielding matte surface appearance. However, in a smooth surface, the facets lie more evenly in the surface plane and their inclinations are low. In such a surface, the reflected rays of light are concentrated around the specular angle [45], leading to a glossy surface appearance.
The angle of incidence ($\theta_i$), the surface roughness ($\beta$), and the wavelength of light ($\lambda$) influence the specular reflectance following the Beckmann and Spizzichino equation [45],

$$L_r = L_i \exp \left[ - \left( \frac{4 \pi \beta}{\lambda} \cos \theta_i \right) \right]$$  \hspace{1cm} (1)

where $L_r$ and $L_i$ is the intensity of the reflected light and incident light at the specular angle, respectively. The reflectance factors ($L_r / L_i$) can be plotted varying the parameter e.g. $\theta_i$ to study how surface roughness dampens the reflectance at specular direction.

For some surface layers which are not homogeneous on a microscale, some rays of light are reflected at the nearly flat outer surface. Other rays of light penetrate deeper inside the inhomogeneous (different refractive index) interior and reemerge after multiple refractions and reflections. The emergence of scattered rays may be near the point of entry with a variety of directions [50]. This type of surface appears as diffuse, flat or matte.

### 3.1.3 Kubelka-Munk theory

The Kubelka-Munk (KM) theory is commonly used to predict the reflectance of turbid media (e.g., in the paper, paint, print, textile, and other color-using industries). Numerous studies in the research literature have explored different aspects of the theory. Discussion of the physical aspects highlighted in this section is presented in the following studies [51, 52, 53, 54].

For a medium that absorbs, emits and scatters light, the KM theory describes the propagation of light using a two-flux approach. Several assumptions are made when applying this theory. A primary assumption is that the light propagates in two opposing directions (Fig. 3-6), and that the variation of flux at any point is linearly proportional to the opposing fluxes [51]. The proportionality constants are the light scattering ($s$) and absorption ($k$) coefficients of media constituents. As a result, the optical properties of the constituent elements can be linked to the bulk properties of the material [53]. Other assumptions are diffuse isotropic illumination, and the presence of an isotropic and homogeneous material. It is assumed that there is no specular reflection, and that the surfaces are plane, parallel, and infinite in
order to discard the boundary effects. The theory assumes the absence of other sources of optical effects, such as polarization, fluorescence, or phosphorescence [52].

Let the reflectance and transmittance of a layer of the medium (Fig. 3-6a) is denoted by $R_0$ and $\tau$. This layer will reflect an amount $IR_0$ and transmit an amount $I\tau$. If the layer is diffusely illuminated by an intensity $J$ from the opposite direction, similarly, the reflected and transmitted amounts of light will be $JR_0$ and $J\tau$. Fig. 3-6b illustrates two fluxes $I$ and $J$ that are denoted by $i(x)$ and $j(x)$ while propagating through the medium in opposite directions. A thin layer inside the medium is $dx$, and the sample consists of a series of layers of equal thickness $dx$. For an ideally black background the reflectance $R_g = 0$, that is in such case, $R_0$ is the reflectance of the sample. In practice, the reflectance of an infinitely thick layer ($R_\alpha$) is considered ($= 0$ so $R_\alpha = R_0$).

![Figure 3-6: (a) The reflectance and transmittance of an ideal layer assumed for KM theory (b) Basic model explaining the Kubela-Munk theory](image)

During the propagation through the layer $dx$, absorption and scattering of the light takes place thus reducing by $(s+k)i\,dx$ and $(s+k)j\,dx$, respectively. The amounts of scattered light in the opposite directions are: $sj\,dx$ and $si\,dx$. These amounts are added to the intensities $i$ and $j$. The total change is given by following differential equations deduced by Kubelka and Munk [53]:

$$-di = -(s+k)i\,dx + sj\,dx \quad (2)$$
$$dj = (s+k)j\,dx + si\,dx \quad (3)$$

The negative sign is used to correctly account the change of light considering that $i$ and $j$ is travelling downwards and upwards, respectively. The Equations 2-3 can be rewritten and integrated
into a range of useful KM equations [55]. In paper technology, the thickness is replaced by the grammage \( w \) (m\(^2\)/Kg) in using the equations to predict the reflectance of the paper. The KM equations are rewritten [45] to calculate the reflectance \( R \) of a paper over a background with reflectance \( R_g \), \( R_0 \) or \( R_\alpha \),

\[
R = \frac{R_a \left( \frac{1}{R_a} - R_g \right) \exp \left[ sw \left( \frac{1}{R_a} - R_a \right) \right] - \frac{R_g - R_a}{R_a} \left( \frac{R_g - R_a}{R_a} \right)}{\left( \frac{1}{R_a} - R_g \right) \exp \left[ sw \left( \frac{1}{R_a} - R_a \right) \right] + (R_g - R_a)}
\]

(4)

\[
R_0 = \frac{R_a \left( \exp \left[ sw \left( \frac{1}{R_a} - R_a \right) \right] \right) - R_a}{\exp \left[ sw \left( \frac{1}{R_a} - R_a \right) \right] - R_0}
\]

(5)

\[
R_\alpha = 1 + \frac{k}{s} - \sqrt{\left( \frac{k}{s} \right)^2 + 2 \left( \frac{k}{s} \right)}
\]

(6)

The light scattering \( s \) and absorption coefficients \( k \) can be calculated by the following equations [45]:

\[
s = \frac{1}{w \left( \frac{1}{R_a} - R_a \right)} \ln \left( \frac{(1 - R_0 R_a) R_a}{(R_\alpha - R_0)} \right)
\]

(7)

\[
k = \frac{s (1 - R_a)^2}{2 R_a}
\]

(8)

where \( R_a \) is the measured reflectance of an opaque pad, and \( R_0 \) is measured with a black background, that is, \( R_\alpha = 0 \).

### 3.2 MODELS OF OPTICAL RADIATION

Specular and diffuse propagations represent two distinct optical radiation phenomena. However, the distinction between these two components depends on the interests and objectives of an application as well as on the measurement device used [56]. In practice, the sum of these components is used to represent the reflectance properties of a real surface. For most surfaces, the simple bidirectional reflectance distribution function (BRDF) can be used where more precise descriptions and specifications of reflectance properties are required [56].
3.2.1 Light reflection model
The image-formation process of an optical system can be most usefully described by reflectance or absorptance. In terms of angular resolution of the system, the BRDF values of reflection along the ray path can be related to specular and/or diffuse reflectance. The specular reflectance corresponds to the values for directions within the angular resolution. The values outside the angular resolution corresponds to the diffuse reflection or scattering [56]. The basic light reflection model is described below, as per the following studies [47, 56, 57].

Fig. 3-7a shows the Zenith/Polar angle $\theta$, which is defined with respect to the surface normal, whereas the Azimuth Angle $\Phi$ is defined with respect to a reference direction. Let $A$ denote the area ($[m^2]$) of the reflecting surface. The spectral radiant flux $\varphi$ i.e., the radiant energy flow per unit time in wavelength $\lambda$, through a point in the surface in a direction $(\theta, \Phi)$, is expressed as follows:

$$\varphi(\lambda, \theta, \Phi) [Wnm^{-1}]$$ (9)

The incident radiant flux per unit area and per unit wavelength is the spectral irradiance $E$:

$$E(\lambda, \theta, \Phi) = \frac{d^2\varphi(\lambda, \theta, \Phi)}{d\lambda dA} [Wm^{-2}nm^{-1}]$$ (10)

The area of the radial projection ($A_{proj}$) of a surface element to the surface of the sphere (with radius $\rho$) is defined as the solid...
angle (unit steradian\( [sr] \)), and the differential solid angle is \( d\omega = dA_{\text{proj}}/\rho^2 \). The solid angle of a full sphere is \( 4\pi \text{ sr} \). The radiant flux per solid angle, per projected area per unit wavelength, is the spectral radiance \( L \),

\[
L(\lambda, \theta, \Phi) = \frac{d^3\varphi(\lambda, \theta, \Phi)}{dA \cos \theta \, d\omega \, d\lambda} \left[ W \text{ m}^{-2} \text{ sr}^{-1} \text{ nm}^{-1} \right] \tag{11}
\]

Equation 11 implies that the spectral radiance is the quotient of radiant flux in a given direction, leaving or arriving at an element of surface (with an area \( dA \)) at a point, and propagated through a cone of solid angle \( d\omega \) in the given direction (Fig. 3-7b).

The Bidirectional Spectral Reflectance Distribution Function (BSRDF)-\( f_r \) models the geometrical reflectance properties as a ratio of differentials:

\[
f_r(\lambda, \theta_i, \Phi_i, \theta_r, \Phi_r) = \frac{dL_r(\lambda, \theta_i, \Phi_i, \theta_r, \Phi_r)}{dE_i(\lambda, \theta_i, \Phi_i)} \left[ \text{sr}^{-1} \right] \tag{12}
\]

where \( dL_r \) is the reflected spectral radiance in the viewing direction, and \( dL_i \) is the spectral irradiance incident to the illumination direction [56]. These two quantities depend on the differential incident flux from direction \((\theta_i, \Phi_i)\) within the differential solid angle as well as the \( dA \) differential element of the surface area. The differential solid angle is \( d\omega = \sin \theta \, d\theta \, d\Phi \) [57]. The incident spectral irradiance on the surface is:

\[
dE_i(\lambda, \theta_i, \Phi_i) = L_i(\lambda, \theta_i, \Phi_i) \cos \theta_i \, d\omega_i \tag{13}
\]

where \( L_i(\lambda, \theta_i, \Phi_i) \) denotes the incident spectral radiance and \( d\omega_i \) denotes the differential solid angle in the direction \((\theta_i, \Phi_i)\). The spectral radiance reflected by the surface is:

\[
L_r = \int dL_r = \int f_r dE_i = \int_{\omega_i} f_r L_i \cos \theta_i \, d\omega_i \tag{14}
\]

Spectral reflectance factors: In practice, the spectral reflectance factor concept is required for the measurements. The spectral reflectance factor is defined as the ratio of the radiant flux at a given wavelength actually reflected by a sample surface to that which would be reflected into the same reflected beam geometry by an ideal perfectly diffuse (Lambertian) standard surface irradiated in exactly the same way as the sample [47, 57].
Assuming that for an ideal perfect diffuse surface, \( f_r = 1/\pi \) [50], the reflectance factor \( r_f \) is defined as follows:

\[
\begin{align*}
\frac{dr}{d\Phi_{\text{ideal \, diffuser}}} &= 0 \\
\end{align*}
\]

where \( d\omega_i = \sin \theta_i d\theta_i d\Phi_i \) and \( d\omega_r = \sin \theta_r d\theta_r d\Phi_r \) are related to the illumination and viewing apertures, accordingly.

**Simplified reflectance model:** A simplified model of the reflectance factor (Equation 15) can be derived for some given surfaces and illumination conditions. A simplification of Shafer's dichromatic model [58] or neutral-interface-reflection [47] model can be used for this purpose. Phenomena such as diffraction, interference, fluorescence, polarization, and refraction are precluded when deriving a simplified model [57]. Assuming a single light source in a simplified reflection model, the spectral radiance on a surface can be expressed in a form that separates the spectral and geometrical factors [47], as for example:

\[
L_i(\lambda, \theta_i, \Phi_i) = L_{i,1}(\lambda) L_{i,2}(\theta_i, \Phi_i)
\]

Please consult Ref. [59] for a practical example where the model (Equation 16) has been used efficiently for 3D visualization of cultural objects. As with Equation 16, separation of geometrical and spectral factors can be assumed in BSRDF:

\[
f_r(\lambda, \theta_i, \Phi_i, \theta_r, \Phi_r) = r(\lambda) g(\theta_i, \Phi_i, \theta_r, \Phi_r)
\]

Similarly, Equation 15 can be rewritten for the reflectance factor, as follows:

\[
r_f(\lambda, \omega_i, \omega_r) = r(\lambda) a_g(\omega_i, \omega_r)
\]

where, \( a_g = \frac{\int_{\omega_i} \int_{\omega_r} g(\theta_i, \Phi_i, \theta_r, \Phi_r) L_{i,2}(\theta_i, \Phi_i) \cos \theta_i d\omega_i \cos \theta_r d\omega_r}{\frac{1}{\pi} \int_{\omega_i} \int_{\omega_r} L_{i,2}(\theta_i, \Phi_i) \cos \theta_i d\omega_i \cos \theta_r d\omega_r}
\]

Two studies [47, 50] can be consulted for more details about the simplification of the term \( a_g \). The simplest model is the Lambertian surface model where \( g(\theta_i, \Phi_i, \theta_r, \Phi_r) \) can be replaced by \( 1/\pi \) in Equation 17 [57].
Theory

\[ f_r(\lambda, \theta_i, \Phi_i, \theta_r, \Phi_r) = \frac{1}{\pi} r(\lambda) \]  

(19)

This simplified model implies that the reflected spectral radiance is the same for all viewing angles \((\theta_r, \Phi_r)\). As a result, the surface appears equally bright and the reflected radiance is isotropic, i.e., \(L_r\) is constant for all directions. The reflectance factor then can be written as follows [57]:

\[ r_f(\lambda, \omega_i, \omega_r) = r(\lambda) \]  

(20)

In this dissertation, all surfaces were assumed Lambertian.

3.2.2 Standard measurement geometry

The measurement geometry specifies the geometric conditions of illumination and viewing of the surface. In graphics arts industry the instruments usually have 45°/0° measurement geometry, and in the pulp and paper industry, the preferred geometry is \(d/0°\) [45]. Another, often followed geometry in various industries is \(d/8°\). However, the geometry plays a large role in measured reflectance for gonioparent objects than diffuse objects like paper or textiles.

In 45°/0° geometry (Fig. 3-8a) the sample is illuminated at an angle of 45° and detector is placed perpendicular to the plane. Print density and colors measurements are made with such instruments. In these instruments, usually polarization filters are used to discard specular reflection that occurs due to surface roughness, although the optical geometry 45°/0° itself acts like a gloss trap [45].

![Figure 3-8: Measurement geometry: (a) 45°/0° (b) d/0°](image-url)
The $d/0^\circ$ geometry (Fig. 3-8b) is recommended by ISO (ISO 2469) for measuring the diffuse reflectance of paper surface. A sphere of a diameter of 150 mm with inside coating of white barium sulfate is used to create the $d/0^\circ$ geometry. The sphere has a hole under which the sample is placed. The detector is placed perpendicular to center of the sample. This instrument has a screen called baffle to prevent the illumination to directly go to the sample or to the sensor. The light diffused inside the sphere strikes the sample. This instrument has gloss traps (usually black matt material) around the opening of the detector to prevent any specular reflection to go to the detector directly from the sample via the coating of the sphere. The reflectance measurement is conducted with respect to a perfect reflecting diffuser. Filters for UV-adjustment should be used according to the recommendations of ISO 2469 standard. In $d/8^\circ$ optical geometry, the diffused light illuminates the sample and detector is placed at angle of $8^\circ$ from the normal.

3.2.3 Reflectance calculation using spectral image
The image formation process involves three fundamental elements: the light source, the object, and the observer (Fig. 3-9). The process begins with a light source which is described by the spectral power distribution $L(\lambda)$ (the relative amount of energy emitted at each wavelength). The light from that source falls on the object’s surface which reflects the light.

![Illustration of spectral image formation](image)

*Figure 3-9: Illustration of spectral image formation. $L(\lambda)$ is the spectral distribution of light from the source, $R(\lambda)$ is the spectral reflectance of the object, and $L(\lambda)R(\lambda)$ is the light reflected towards the observer.*
The surface reflectance function \( R(\lambda) \) defines the fraction of light reflected by the surface. The color signal can be defined as the multiplication of the signals \( L(\lambda) \) and \( R(\lambda) \), which eventually leads to the experience of color [48]. The reflected light \( L(\lambda)R(\lambda) \) reaches to the observer (e.g. a camera) that intercepts according to the spectral sensitivity functions of the channels \( C_i(\lambda) \).

Reflectance is independent of the illumination and the observer. Due to this property, spectral reflectance can be used for object characterization and analysis in many color-related applications. Since most instruments measure the total radiance reflected from the surface, it is essential to calculate the reflectance factors. The obtained reflectance spectra can then be used for purposes such as computing the signal detected by any observer in an arbitrary illumination, calculating standard color coordinates, or determining spectral filters [60].

In spectral imaging systems, a certain wavelength range \( (\lambda) \) is divided into \( n \) discrete and finite number of bands. In these systems, each channel or detector detects a signal corresponding to a specific band. The channel is realized by the spectral sensitivity of the entire spectrum given the full width at half maximum (FWHM) inside the specific band [61]. If any arbitrary point on the measured surface has a reflectance \( R(\lambda) \), the signal detected by the observer at channel \( i \) (assuming the number of channels is also \( n \)) is:

\[
d_i = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} L(\lambda)R(\lambda)C_i(\lambda) d\lambda + \eta_i
\]  

(21)

where \( C_i(\lambda) \) is the \( i \)-th channel’s spectral sensitivity function, and \( \eta_i \) is the measured dark noise. Here, all the functions are discrete \( n \)-dimensional vectors \( l, r, c \in \mathbb{R}^n \), so, for example, the reflectance can be expressed in vector form as:

\[
r = [R(\lambda_1), R(\lambda_2), \ldots, R(\lambda_n)]^t
\]  

(22)

where \( t \) is used to indicate the transpose operation. The matrix notation of Equation 21 is [60]:

\[
d_i = w_i^t r + \eta_i
\]  

(23)

where,

\[
w_i = \text{diag}(l) c_i
\]  

(24)
That is, \( w_i \) captures the joint spectral effect of the illumination and sensitivity of the \( i^{th} \) channel. The vector \( d \in \mathbb{R}^n \) of the signals detected by all the channels is:

\[
d = W^t r + \eta_{dark}
\]

where \( W \) is a \( n \times n \) matrix with \( w_i \) as the columns, and the vector \( \eta_{dark} \in \mathbb{R}^n \) comprises the dark noise \( \eta_i \) of each channel. In practice, a standard white reference is measured, and if \( r_{white}(\lambda) \) is the reflectance of standard white in the same spectral range, then the detected signal is:

\[
d_{white} = W^t r_{white} + \eta_{dark}
\]

According to that definition, the ratio of the reflected light from the measured surface in comparison to the reflected light from a white reference under identical specified geometric conditions is the reflectance, \( r \), given by:

\[
r = \frac{d - \eta_{dark}}{d_{white} - \eta_{dark}}
\]

Note that in this thesis, we have used Equation 27 consistently for all measurements to calculate reflectance factors of the object under investigation.

### 3.2.4 Beer-Lambert’s Law

A transparent medium can be quantitatively described by transmission and absorption using the Lambert and Beer laws [62]. Lambert’s law states that the same fraction of incident monochromatic radiation will be transmitted through layers of equal thickness and of the same material. In an absorbing medium, the transmittance of light varies exponentially. Beer’s law states that the absorption of light is proportional to the number of absorbing particles along its path. That is, for a given path length, the amount of transmitted light reduces proportional to the light absorbing particles. Mathematical formula [62] expressing Beer-Lambert’s law is,

\[
A = \alpha \varepsilon c = \log \frac{I_0}{\tau} = \log \frac{I_0}{I_T}
\]

where, \( A \) is the absorbance, \( I_0 \) is the incident light intensity, \( I_T \) is the transmitted light intensity, \( \tau \) is the transmittance of the
medium, $\alpha$ is the absorption coefficient, $\varepsilon$ is the length of light path, and $c$ is the concentration of light absorbing particles.

### 3.3 Imaging Systems

The discrete grid elements of imaging sensors have fixed sizes in the image space, with varying sizes in the object space [57]. The focal length and distance to the object determine the spatial area covered by a single sensor element. Let $\Omega = [\lambda_{min}, \lambda_{max}]$ denote a range of wavelength bands in a particular discussion. In an imaging system, the sensor uses its spectral response function to sample the reflected EM spectrum over $\Omega$. FWHM is used to specify the spectral bandwidths of spectral response functions. A monochromatic system has one spectral band within $\Omega$, whereas a multispectral system has several narrow and discretely located bands in the region $\Omega$. A hyperspectral system may have hundreds of bands located over a contiguous wavelength spectral range in the region $\Omega$. However, the number of bands defining multi- or hyper-spectral systems is not fixed. We use the term spectral to cover both systems. Since the RGB sensor systems cover broad bands in the entire VIS range, these systems are commonly considered as a separate class tailored for color photography [57].

#### 3.3.1 Imaging technologies

The imaging process involves the main components as has been described previously (Fig. 3-9). Remember that we denote the spectral power distribution of the illuminant by $L(\lambda)$, the surface reflectance by $R(\lambda)$, the $i$-th sensor’s spectral sensitivity by $C_i(\lambda)$, and the dark noise by $\eta_{dark}$. For a fixed geometry, the signal detected at a point $(x, y)$ in a $n$-band sensor system $(i = 1, 2, \ldots, n)$ is:

$$d_i(x, y) = \int_{\lambda_{min}}^{\lambda_{max}} L(\lambda) R(x, y, \lambda) C_i(\lambda) d\lambda + \eta_{dark}$$

(29)

Here, it is assumed that the $C_i(\lambda)$ spectral sensitivity functions include the joint effect of the sensors’ quantum efficiency (spectral sensitivity), and transmission of the optics and filters.
The \( \{d_i\}_{i=1}^n \) analog signals are converted to electronic signals and are normally quantized using between 8 and 16 bits.

Common RGB devices have three broad optical bandwidths and the detector integrates all the spectral information into a single value. The \( \{d_i\}_{i=1}^3 \) values are termed RGB values. Fig. 3-10a shows the spectral sensitivity functions of the RGB channels of an RGB camera. These functions attempt to mimic human perception so that the rendered colors match as well as possible with what humans observe [60]. In some devices, color filter arrays are used for imaging (Fig. 3-10b). In this case, the response of a particular position is captured in some channels, and neighborhood interpolations are performed to obtain values for the same position in other channels [57].

Figure 3-10: RGB imaging: (a) Spectral sensitivity functions of the camera embedded in a Nokia 1520 phone (b) Color filter arrays

Spectral imaging devices fall into three categories: point measurements, wavelength scan imaging, and line scan (push-broom) imaging. A spectrometer is an example of a point measurement device where dispersive optics (e.g., diffraction grating or prisms) are used for light dispersion. Fig. 3-11 illustrates how diffraction grating disperses the light emitting from a relatively small area. The dispersed light is projected onto the surface of a photodetector array that records the optical properties as a function of the wavelength bands [63]. This system does not provide any spatial information.

The band-sequential technique [64] is one of a number of techniques used for wavelength scan imaging. In this technique, multiple measurements are made with the aid of a set filters and a monochromatic camera. Fig. 3-12a illustrates the operation of
Figure 3-11: Schematic of dispersive element based point measurement system

a spectral imaging system based on a filter wheel. A grayscale image is captured for each filter. The bandwidth of a filter determines the range of wavelengths included in each scan [63]. The number of acquired spectral channels is equal to the number of filters in the wheel. Liquid crystal tunable filters (LCTF) (Fig. 3-12b) are one of the most widely used variable filters, improving the convenience of wavelength scan imaging. This technology has no mechanical parts and switches times between wavelengths quickly. The main component is a polarizable liquid crystal positioned between two linear polarizers. When voltage is applied, a narrow band of wavelengths passes through the LCTF stack [63].

Figure 3-12: Schematic of spectral imaging system based on : (a) rotating filter wheel (b) LCTF

In the line scanning (push-broom) system, a sequence of scans is performed to construct a spectral image. Fig. 3-13a shows that the spectra are acquired from one line of a sample at each scan. In order for this to happen, either the object or the camera system has to move. Fig. 3-13b shows that the guided light is focused on the slit that passes the light on a prism-grating-prism (PGP) element. The PGP disperses the light into spectral components

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and a matrix detector detects them. The spectra are aligned along the spectral axis of the detector [63].

Figure 3-13: Schematic of line scanning imaging system: (a) Set-up (b) principle of operation

3.3.2 Used imaging systems and processing
In all the experiments carried out, we used 45/0° geometry to measure the samples. In general, we followed the standard procedure to correct dark current and electronic gain for each pixel of the sensor for each individual channel/band. The electronic gain was characterized by capturing images of (diffuse) standard reference white ($I_w$) under the same illumination. Note that in the case of microscopic imaging, the white plane of reference was set slightly off focus to avoid non-homogeneity of the surface structure [64]. The illumination was turned off and the lens cap was on during capture of the dark current image($I_D$). If $I_k(x,y)$ denotes the acquired image for each channel/band $k$, the correction for dark current and CCD gain was:

$$I(x,y) = \frac{I_k(x,y) - I_D(x,y)}{I_w(x,y) - I_D(x,y)}$$

(30)

3.3.2.1 Microscopic imaging
The samples studied in Papers I and II were measured by three different microscopic RGB and/or spectral imaging systems. Fig. 3-14 presents a common schematic diagram of the imaging systems. The systems have an optical microscope setting that magnifies the surface of the sample. The light sources can optionally be used to illuminate the sample from the upside (reflectance mode) and/or the downside (transmittance mode). The reflected (or transmitted) light from the sample goes through
the microscope to a digital monochrome CCD/RGB/spectral camera.

![Diagram of microscope-camera set-up](image)

**Figure 3-14: General diagram of the microscope-camera set-up.**

**RGB imaging by co-registered RGB/spectral system:** RGB images of the samples in Set-1 (Paper I) were acquired by the microscopic imaging system (Oden scanner) installed in the Media and Information Technology (MIT) laboratory in Linköping University. The system was specially designed [65, 66, 67] to study different aspects of halftone prints performing trichromatic and spectral imaging. Note that the RGB images of the samples were stored directly as radiance images. As a result, no correction was applied for non-linearity.

This setup has a monochrome CCD camera with a 12-bit dynamic range at the $0^\circ$ position. A tungsten halogen lamp provides illumination through optical fibers at a $45^\circ$ angle of incidence. The filters are mounted in a filter wheel in front of the light source to capture the color images sequentially. The filter wheel also contains a set of interference filters to cover the visible spectrum with equally-spaced pass bands. Two studies [68, 64] provide details of the characterization, calibration, and the spectral properties of the illumination, camera, and filters.

**RGB imaging by a professional microscope-RGB camera system:** The samples of Set-2 (Paper I) were imaged by a professional imaging system in a commercial pulp and paper research company, MoRE at Örnsköldsvik, Sweden [69]. The system, which is used professionally to study fibers and surfaces of paper products, consists of a general light microscope with an RGB camera...
attached to it. A built-in controllable light source precisely illuminates the surface of the prints. We did not have access to the technical configurations of the imaging model. The supplied RGB image was in standard RGB (sRGB) format. The following equations were used to convert gamma-corrected sRGB values back to linear values [70]:

\[ I_{\text{linear}} = \frac{I}{1/2.92}, \text{ if } I \leq 0.04045 \]
\[ I_{\text{linear}} = \left( \frac{(I + 0.055)/1.055}{2.4} \right)^{1/2.4}, \text{ if } I > 0.04045 \]

**Spectral imaging:** The colorimetric and spectral images of the samples (Paper II) were acquired by a system consists of an optical microscope (Nikon Eclipse MA200) and a CRi Nuance spectral imaging camera (model N-MSI-EX) in the University of Eastern Finland (Spectral Color Research Lab.). The halogen lamps illuminated at an (approx.) 8° angle, while the detector was at 0°. The selected spectral bands ranged from 420 nm to 700 nm in steps of 10 nm. The 12-bit depth camera stored images as straightforward radiance images. Fig. 3-15 shows the dark current and exposure time corrected and normalized spectral transmittance curves [71] of LCTFs used in the imaging system.

![Figure 3-15: Normalized transmittance curves of the LCTFs.](image)

The corresponding RGB image of each sample was captured at the same time and under the same conditions as the spectral radiance image. The control software offers the option for RGB imaging. However, no information is available regarding the mechanism of RGB sampling. The RGB colors of the samples were in accordance with the original samples, there were no
pseudo colors. Since there was no additional filter and the speed was very fast, the author assumes the system tunes LCTFs to cover the typical broad optical bands of RGB imaging. Fig. 3-16 compares the reflectance curves of bare paper (unocated) and full-tone cyan measured by spectral imaging and a standard *Gretag Machbeth Spectrolino* spectrophotometer with UV filter.

![Reflectance curve comparison](image)

*Figure 3-16: Comparison of measured reflectance of bare paper and fulltone cyan ink. Solid lines are measured by spectral camera and broken lines by standard Gretag Macbeth Spectrolino spectrophotometer.*

### 3.3.2.2 Spectral imaging with line scanning system

The samples studied for Paper III and IV were measured by a spectral line scanning camera system (*Specim*, Oulu, Finland) that has two cameras covering the VIS/NIR (400–1000 nm) and SWIR (1000–2500 nm) spectral wavelength range, independently. Tables 1 and 2 list the specifications of the cameras and the measurement conditions. Halogen lamps mounted in a separate casing that moves with the camera were engaged to illuminate the samples. The imaging procedure generated three-dimensional (3D) cubes wherein the spatial information was in 2D and the spectral information was in the third dimension. The internal shutter of the camera was closed to acquire a dark image, and a Spectralon® reference white plate was measured for the reference white image.
Table 1: Measurement specifications for VIS/NIR range

<table>
<thead>
<tr>
<th>Camera</th>
<th>Zyla 5.5 sCMOS; Andor Tech., Belfast, UK</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lens</td>
<td>V18.5 – f/2.4 091101 Specim Ltd.</td>
</tr>
<tr>
<td>Spectrograph</td>
<td>ImSpector V10E; Specim, Spectral Imaging Ltd.</td>
</tr>
<tr>
<td>Data form</td>
<td>Spectral radiance, 386-998 nm at 3 nm intervals</td>
</tr>
<tr>
<td>Standard white</td>
<td>Spectralon® reference plate (Specim Ltd.)</td>
</tr>
<tr>
<td>Light source</td>
<td>2 set halogen lamps (35 W each), 45/0° geometry</td>
</tr>
<tr>
<td>Spatial resolution</td>
<td>6.5 micrometer</td>
</tr>
<tr>
<td>Sample distance</td>
<td>395 mm</td>
</tr>
<tr>
<td>Exposure time</td>
<td>9.1 ms</td>
</tr>
</tbody>
</table>

Table 2: Measurement specifications for SWIR range

<table>
<thead>
<tr>
<th>Camera</th>
<th>LVDS-100; Specim, Spectral Imaging Ltd.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lens</td>
<td>OLES15-f/2.0 052301 Specim Ltd.</td>
</tr>
<tr>
<td>Spectrograph</td>
<td>ImSpector N25E; Specim Spectral Imaging Ltd.</td>
</tr>
<tr>
<td>Data form</td>
<td>Spectral radiance, 933-2538 nm at 6 nm intervals</td>
</tr>
<tr>
<td>Standard white</td>
<td>Spectralon® reference plate (Specim Ltd.)</td>
</tr>
<tr>
<td>Light source</td>
<td>2 set halogen lamps (35 W each), 45/0° geometry</td>
</tr>
<tr>
<td>Spatial resolution</td>
<td>30 micrometer</td>
</tr>
<tr>
<td>Sample distance</td>
<td>380 mm</td>
</tr>
<tr>
<td>Exposure time</td>
<td>1.6 ms</td>
</tr>
</tbody>
</table>
3.4 COLOR PRINTING

Paper, which is the most common media used for printing, is a three-dimensional network consisting of fibers, fillers, and additives to improve the optical properties [72]. The paper receives inks that create the color appearance, and used as the background for ink reflectance. The quality of the print is determined by the paper’s optical properties and its interaction with the ink [73, 74, 75]. The paper coating or surface treatment depends on the target print technology. Ink absorption and spreading occur when the ink is applied to the paper, leading to physical dot gain [72]. The paper’s properties and color prediction models (CPM) are considered to transform the color values into process inks [76]. The printing technology transfers the inks to the substrate as the next operational task.

3.4.1 Printing technology

In this dissertation, offset and electrophotography technologies were mainly used to prepare the samples. Electrophotography is a variety of digital printing technology. Fig. 3-17 shows that in offset technology, a printing plate is sequentially dampened by water and ink. As the image area is only receptive to ink, the plate transfers the inked image to a rubber blanket. Finally, the blanket transfers that inked image to the paper. In a multi-color print production, the steps are followed sequentially for each ink [76].

![Illustration of a conventional (offset) printing process](image-url)

*Figure 3-17: Illustration of a conventional (offset) printing process [77].*
Fig. 3-18 describes the principle behind electrophotography printing technology, wherein the hardware typically consists of a drum. The drum is made of a highly photoconductive material reactive to light. The corona wire electrically charges the drum. A laser beam discharges specific areas on the drum to form the target image. Positively charged toner is attracted and twigs solely to the image pattern. The paper also becomes electrically charged and receives the pattern of the toner while passing by the drum on a belt. Finally, the toner particles are melted into the paper by the fuser [76]. The HP Indigo printers use liquid electro photographic ink to print images with high resolution, uniform gloss, sharp edges, and very thin image layers [78].

Figure 3-18: Illustration of the digital electrophotography printing process [77].

3.4.2 Halftoning
Halftoning is an important part for image reproduction by devices that use a limited number of colors. The quality of a print is substantially influenced by dot gain that is greatly dependent on halftoning. A continuous tone digital image is discretized into a bitmap by halftoning (also known as screening). The average color of an image area is rendered by printing ink dots according to the halftone cell pattern. Variations of the gray levels are produced by changing the ink depositions in a specific location. A ‘1’ in a bitmap image instructs the binary printer to print a black dot and a ‘0’ instructs to skip the position. The average tone of corresponding area in the original image is represented by the fractional area that is covered by the ink in a halftone cell. For
color printing, this transformation is usually accomplished for each of the color channel that the printing device uses.

The screen frequency (halftone cells/lines per inch (\(lpi\))) and print resolution (number of dots per inch (\(dpi\))) determine the number of reproducible gray levels ((\(dpi/lpi\))^2 +1) of a halftone image. As shown in Fig. 3-19, each halftone cell is divided into a number of micro dots. The size of the ink dot in Fig. 3-19a is 2x2 representing the gray tone of 4/64, and the other cell represents the gray tone of 20/64. As a result, total 65 (8^2+1) different gray tones can be represented by an 8x8 halftone cell.

Amplitude modulation (AM) and frequency modulation (FM) are the two basic strategies for applying the halftone methods [79]. Fig. 3-20 shows two halftone cells that represent the same gray tone. In AM halftoning, the size of the ink dots are varied while their spatial frequency are kept constant (Fig. 3-20a). That is to represent darker tones the size of the dot is increased. In the FM technique, the size and shape of the dots remain constant, but the frequencies (the number of micro dots) are varied (Fig. 3-13b).

In general, most of the known FM techniques (e.g. error diffusion) don’t use halftone cells to build the final image. Therefore, instead of \(lpi\), only the print resolution term \(dpi\) is used in specifying FM resolution. In contrast to AM techniques, generally the FM techniques do not produce any ordered
structures. The FM technique is a better choice when details of an image is required to reproduce. On the other hand, AM performs better for areas where the variation of tone is slow, because in such regions the FM techniques generally yield noisy impression.

**Halftoning Methods**
The details of various halftoning methods can be found in [80]. Here, a brief description of few halftoning methods is presented that are relevant to samples reparations for the study in Paper I-II. It is assumed that the original image is scaled between 0 to 1.

*Threshold halftoning:* A threshold matrix is used in this technique to map the tonal range of the original image to the halftones. The following equations describe the technique.

\[
H(i,j) = \begin{cases} 
1 & \text{if } I(i,j) \geq T(i,j) \\
0 & \text{if } I(i,j) < T(i,j)
\end{cases}
\]

where \(H, I\) and \(T\) denote the halftoned image, the original image and the threshold matrix, respectively. The pixel value of \(H\) at each position \((i,j)\) is compared to the corresponding position in \(T\). If the pixel value is greater than or equal to the threshold value, a ‘1’ (ink dot), else a ‘0’ (no ink) is assigned there in \(H\). If the size of \(T\) is smaller than \(I\), then periodic repetition is made in both directions to make the \(T\) to be the same size of \(I\).

Ordered dithering is a common class of threshold halftoning techniques. This class is divided into two parts: clustered dot and dispersed dot. The threshold matrix \(T\) in clustered dot dithering is arranged in way so that the final halftone dot is a cluster of black microdots. On the other hand, the final black microdots are dispersed in dispersed dithering.

*Error Diffusion:* Floyd and Steinberg introduced the error diffusion halftoning technique in the mid-1970s. This dithering technique operates on a neighborhood of currently processing pixels. Fig. 3-21 illustrates the operations.
The algorithm operates on each pixel position in the original image $I$. The value of each pixel in $I$ is compared to a threshold that is normally set as 0.5. If the pixel value is greater than the threshold, ‘1’ is assigned to $H$, else ‘0’ is assigned. By doing this an error occurs which is the difference between the pixel value of the same position of $I$ and $H$. This error is diffused among the unprocessed pixels. To which pixel and how the error is diffused is determined by an error filter [80].

Fig. 3-22 shows the error filter known as Floyd and Steinberg error filter. This filter weights the error occurred at the position $(i,j)$ (shown by a black box in Fig. 3-22) by 7/16 and adds to the pixel at the location $(i+1,j)$. The filter weights the same error by 1/16 and added to the pixel value at location $(i+1,j+1)$. This way the filter diffuses the error. After finishing the diffusion of error at the location $(i,j)$, the pixel value at the next position is compared to the threshold and the same process continues until all pixels have been processed.

**Figure 3-22: Floyd and Steinberg error filters**

### 3.4.3 Dot gain
Ink is placed on the paper surface by the printer and it is expected to have uniform density. However, the ink spreads over the surface to some extent and penetrates into the paper’s structure (Fig. 3-23) [72]. The scale of the spreading and penetration
depends on the type of printing technology, ink, and paper grade [81]. The natural consequence of this is a decreased density towards the dot edge [82].

![Image](image1.png)

Figure 3-23: (a) Schematic diagram of ink spreading and penetration [76], and (b) real case of ink absorption in coated paper [77].

The ink and paper components may mix together, especially in surrounding the dots, because of the low thickness and uneven capillary penetration [72, 75]. For example, Fig. 3-23b illustrates the ink absorption in a highly magnified cross-sectional image of a square patch printed by an HP Designjet 10ps inkjet printer with water-based dye inks. Fig. 3-24a shows the ink spreading effect in the case of pigment-based cyan ink on uncoated office paper printed with a modern inkjet printer (Canon imagePrograf iPF 6000). The true fractional ink area covered by the solid ink may increase (or decrease), which is known as physical or mechanical dot gain.

![Image](image2.png)

Figure 3-24: (a) Top view of microscale dots of ink, and (b) light interactions with ink and paper [77].

Optical dot gain, which is also known as the Yule-Nielsen (YN) effect, is the phenomenon by which the printed dots are perceived as larger and darker [72, 81, 83]. This is due to various light interactions with the ink and paper, as schematized in Fig. 3-24b. The non-inked paper close to the solid ink boundary
receives the tint of the ink due to the type of event depicted at ‘a’ and ‘d’ [72]. Arrow ‘a’ indicates that the light entering the unprinted part of the paper scatters laterally before being absorbed by the ink on its way out under the edge of the ink film.

**Dot gain estimation:** The overall dot gain can be estimated by reflection densitometer, spectrophotometer, or microscopic image analysis [76]. The conventional practice is to estimate the effective ink area or total dot gain through the performance optimization of the MD model [84, 65]. The optimization criterion is to minimize the difference between the spectral root mean squared (sRMS) error of the measured (\(r_{\lambda, meas}\)) and the predicted (\(\hat{r}_\lambda\)) reflectance. The final expression in matrix form is shown using the least squares sense [84]:

\[
a_{eff}(a) = dr_{\lambda, meas} dr_{\lambda, I}^{-1} (dr_{\lambda, I} dr_{\lambda, I}^{-1})^{-1}
\]

Here, \(dr_{\lambda, meas} = r_{\lambda, meas}(a) - r_{\lambda, P}\) and \(dr_{\lambda, I} = r_{\lambda, I} - r_{\lambda, P}\), \(r_{\lambda, P}\) and \(r_{\lambda, I}\) are the measured spectral reflectance of the bare paper and fulltone ink, \(a_{eff}\) is the effective coverage, \(a\) is the nominal coverage. The total dot gain (\(\Delta a_{tot}\)) is:

\[
\Delta a_{tot}(a) = a_{eff}(a) - a
\]

A set of single colorant patches with varying nominal coverage (ranging from 0% to 100% at a reasonable gap) is used to characterize the dot gain. The dot gain characteristics curve of a particular print set up helps to correct the ink compensation that is applied prior to halftoning. The interpolation of the curve corresponds to the dot gain or effective coverage for any arbitrary nominal coverage. Fig. 3-25 demonstrates the effective coverage curves for offset prints on glossy coated paper as classified by the FM or AM method. The curves were measured using the image analysis method described in this dissertation. The arrow indicates that in order to obtain 60% effective ink coverage, the bitmap image should have a nominal coverage of around 51%, given AM halftoning.
A color prediction model (CPM) predicts the reflectance of a printed surface, given the relative coverages of the ink and paper. The inputs of a forward CPM are the fractional coverages of ink (e.g., RGB, CMY) and the outputs are the coordinates in a device-independent color space (e.g., CIE XYZ, CIE LAB). The CPMs are trained through printing and measuring samples in variations of the substrates, the printers, halftoning, and the inks. After training, the inverted model estimates the amount of RGB or CMY colorant coverages to print a color associated with a given coordinate in a device-independent color space [36].

Ref. [85, 36] can be consulted for excellent review of the state of the art CPMs. The principle behind first principal models (e.g., Kubelka-Munk, Clapper-Yule, Probabilistic) is to study the light reflection processes with an emphasis on better understanding the physics behind those processes. On the other hand, the regression-based models (e.g., Murray-Davies, Neugebauer, Yule-Nielsen) exhibit a better prediction performance as the parameters are optimally fitted to a set of measured data. The regression-based models support printer characterization and calibration by means of printing and measuring large numbers of samples [36, 86].

In this dissertation, the Murray-Davies (MD) model was studied as the base model due to its simplicity and sound theoretical background. Furthermore, current successful models
such as the Yule-Nielsen and Neugebauer models are based on this model. In fact, many useful models are actually direct expansions of the monochrome MD model for multiple colorants [36]. In this section, brief descriptions of the relevant models are provided.

### 3.5.1 Murray-Davies model

The basic MD formula (Equation 34) equates the reflectance to the sum of the light reflected off various areas of a print in order to maintain the conservation of energy principle. The equation relates the reflectance of a monochrome halftone print with arbitrary nominal ink coverage ($a$) to the reference reflectance of unprinted paper ($R_P$) and full ink coverage ($R_I$). This model can be interpreted as a linear interpolation between $R_I$ and $R_P$, as weighted by the corresponding fractional area coverages.

\[
\hat{R} (a) = a R_I + (1 - a) R_P
\]  

(34)

The symbol $\lambda$ is added to the subscript of the variables to indicate the spectral reflectance and hence the spectral version of the model is presented in vector forms in Equation 35.

\[
\hat{r}_{\lambda} (a) = a r_{\lambda,I} + (1 - a) r_{\lambda,P}
\]  

(35)

Here, the point to be noted is that this model assumes the reflectance of unprinted paper and full tone inks to be uniform and constant. Therefore, in practice, a large difference is observed between the predicted and the measured reflectance due to the dot gain phenomenon. The prediction accuracy of the MD model can be improved significantly if the effective coverage is used instead of the nominal coverage. This model is oft-followed in industry for estimating the effective area or total dot gain by minimizing the difference between the sRMS error of the measured and the predicted reflectance [36, 65, 66].

### 3.5.2 Expanded Murray-Davies Model

The base MD equation was investigated by Arney, Engeldrum and Zeng [87] accounting the change of reflectance of halftone image components but maintaining the linear additivity of reflectance. They modeled the variable reflectance of ink ($\hat{r}_{\lambda,I}$) and paper ($\hat{r}_{\lambda,P}$) as a function of arbitrary nominal coverage ($a$):
Use of Reflectance Measurements to Study Turbid Media by Imaging

\[ \hat{r}_{\lambda,i} (a) = r_{\lambda,0} \left( 1 - (1 - \tau_{\lambda,i}) \alpha_{\text{eff},i} \right) \left( 1 - (1 - \tau_{\lambda,i}) \alpha_{\text{eff},i} \right) \]

\[ \hat{r}_{\lambda,p} (a) = r_{\lambda,0} \left( 1 - (1 - \tau_{\lambda,i}) \left( 1 - \alpha_{\text{eff},p} \right) \right) \left( 1 - (1 - \tau_{\lambda,i}) \left( 1 - \alpha_{\text{eff},p} \right) \right) \]

where \( r_{\lambda,0} \) is the measured spectral reflectance of bulk paper, \( \tau_{\lambda,i} \) is the spectral transmittance of fulltone ink which is equal to \( \sqrt{\hat{r}_{\lambda,i} / r_{\lambda,0}} \), \( \alpha_{\text{eff},i} \) is the effective coverage of arbitrary nominal ink coverage \( i \), \( \bar{w} \) is an empirical parameter accounting the effect of light scattering, \( \bar{v} \) is an empirical parameter for the distortion of dot edge, and \( \alpha_{\text{eff},p} \) is the corresponding area coverage of the paper between dots. The calculated variable reflectances (\( \hat{r}_{\lambda,i} \) and \( \hat{r}_{\lambda,p} \)) are fed in the MD formula to calculate the overall halftone reflectance as:

\[ \hat{r}_{\lambda} (a) = a \hat{r}_{\lambda,i} (a) + (1 - a) \hat{r}_{\lambda,p} (a) \]

Note that though the calculated \( \hat{r}_{\lambda,i} \) and \( \hat{r}_{\lambda,p} \) substantially differ from experimental data but the predicted halftone reflectance \( \hat{r}_{\lambda} \) fits with the measured reflectance better than YN model [88].

3.5.3 Other relevant models

Yule and Nielsen (YN) model: Yule and Nielsen proposed a nonlinear relationship with a power function to modify the MD formula based on an analysis of the light penetration and scattering [36] as:

\[ \hat{r}_{\lambda} (a) = \left( a_{\text{eff}} (a) \right)^{\frac{1}{\bar{w}_{\lambda,i}}} + \left( 1 - a_{\text{eff}} (a) \right) \left( \frac{1}{\bar{w}_{\lambda,p}} \right)^{n} \]

Note that in order to account for the physical dot gain, the nominal coverage \( a \) is replaced with the effective area coverage \( a_{\text{eff}} \) in Equation 39. The factor \( n \) (known as the YN n-factor) was proposed to account for the light scattering effect (i.e., optical dot gain) [86].

The YN n-factor is empirically determined so as to best fit with the experimental data [89, 90]. The simple process involves plotting the \( n \) value against the error metric in an iterative process or performing a non-linear optimization to identify the best value. The range of the value for the \( n \)-factor is uncertain: negative to infinity [91]. This model improves the prediction
accuracy, but at the cost of losing the elegance of the energy conservation principle. Furthermore, the $n$-factor only explains the optical dot gain in limited cases, as reported in many investigations [86, 92, 93, 94].

Spectral Neugebauer model: The original Neugebauer model predicts the CIE-XYZ tri-stimulus values of a halftone color patch as a linear contribution to the tri-stimulus values, with fractional area coverages of each ink. Instead of tri-stimulus values, this model can also predict the reflectance of a color halftone image using similar equations.

The model is a straightforward extension of a monochrome MD equation based on three process colors: cyan, magenta and yellow (CMY). The reflectance factor of fulltone prints of the process colors and their possible combinations are termed as the Neugebauer primaries. For CMY printers, the eight Neugebauer primaries comprise: no color (bare substrate), three-color overlaps (black), two-color overlaps (red, green, blue), and single separations (cyan, magenta, yellow). The model linearly combines the reflectance factors of all the primaries and the corresponding fractional coverage in order to measure the contribution of each primary to the overall reflectance [36]:

$$\hat{r}_\lambda = \sum_i a_i r_{\lambda,i}, \quad \sum_i a_i = 1$$

where $r_{\lambda,i}$ denotes the spectral reflectance of the $i$-th primary at full coverage, and $a_i$ is the fractional area coverage of the $i$-th primary. Typically Demichel’s Probabilistic equations [36] are used to estimate the fractional coverages of the primaries, if the halftones dots are randomly distributed.

The first step to evaluate the Demichel’s equations is to determine the effective coverages of the three primaries: cyan ($a_{eff,c}$), magenta ($a_{eff,m}$) and yellow ($a_{eff,y}$). The characterized dot gain curves of each process ink can be used for determining these values. In the second step the actual effective coverage of each primary in a multicolor print is estimated using Demichel’s equations:

$$a_{\text{white}} = (1 - a_{eff,c})(1 - a_{eff,m})(1 - a_{eff,y})$$
These values are fed into Equation 40 with the measured spectral reflectance of the fulltone primaries to calculate the overall reflectance. The same assumption is made regarding the consistency of ink and paper reflectance as with the MD model. This model can be explained as performing trilinear interpolations across the reflectance space of the printer [36]. The spectral reflectances of the primaries are the nodes of this space (Fig. 3-26). As with the MD model, the model takes as input the distances along the colorant axis and the spectral reflectance of the primaries. In the case of multiple colorants, Fig. 3-26 illustrates that the weight for the spectral reflectance of each colorant is the area of the respective rectangle, which is defined by the boundary of the effective coverage. The performance of this model is also limited owing to optical dot gain, which invalidates the assumed linearity between reflectance and ink coverage.

![Graphical representation of Neugebauer model. The area of respective rectangle is the weight for each primary (redrawn after [36]).](image)

Yule and Nielsen Modified Spectral Neugebauer model(YNSN): Yule and Nielsen improved the Neugebauer model by accounting for optical dot gain, which is a non-linear phenomenon caused by light scattering. Later, Viggiano showed that incorporating
spectral reflectance instead of CIE-XYZ tri-stimulus values yields greater accuracy [85]. The modified equation introducing the empirical parameter \( n \) is as follows:

\[
\hat{r}_\lambda = \left( \sum_i a_i r_{\lambda,i}^{-\frac{1}{n}} \right)^n, \quad \sum_i a_i = 1
\]  \( (42) \)

The value of \( n \) can be determined by an iterative approach minimizing the sRMS difference between the predicted and measured reflectance of a set of samples. Although the YNSN model is frequently used for printer characterization, the relation of \( n \)-values with respect to the printing condition is still a matter for debate. This has generally been identified with the ink spreading phenomenon [95].

**Ink spreading enhanced YNSN model:** When used with the YNSN model, a new ink-spreading model, proposed by Hersch and Crete [95], notably improves the accuracy of spectral reflectance prediction of color prints. This technique incorporates more accurate estimations of ink coverage into the YNSN model. As a result, the basic ink spreading assessment method was improved, based on the fact that the amount of ink spreading depends on whether the ink is alone on the support or superposed with other inks [85]. This superposition-dependent ink spreading assessment method estimates effective dot surface coverage more accurately.

Fig. 3-27 shows the workflow diagram of the model. In this workflow, for each superposition condition, at first an ink-spreading curve is determined aiming at mapping the nominal dot coverage \((c_0, m_0, y_0)\) to the enhanced dot coverage \((c', m', y')\). The curve is obtained minimizing the sum of square differences between measured reflection spectra and reflection spectra predicted by the YNSN model. The nominal to enhanced surface coverage curve is obtained by a weighted average of the characteristics ink-spreading curves. Equation 43 shows the weighted conversion as an example for cyan ink. The enhanced coverages are plugged into Demichel’s equations to calculate the effective coverage. The effective coverage are used with a near optimal \( n \) value in Equation 42 to predict the reflectance.
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\[ c' = (1 - m)(1 - y)f_c(c_0) + m(1 - y)f_{c/m}(c_0) + (1 - m)yf_{c/y}(c_0) + myf_{c/my}(c_0) \]  \hspace{1cm} (43)

**Figure 3-27: YNSN model with enhanced ink spreading functions (redrawn after [85])**

### 3.5.4 Engeldrum’s model

P.G. Engeldrum [38] proposed models to characterize the changes in the CIE tristimulus values (TSVs) of paper and ink in a halftone print. A new term was introduced, namely the limiting value \( T_{\text{limit}} \), which refers to the TSVs of paper when the coverage approaches one or the TSVs of the dots when the coverage approaches zero. If the TSV \( (X, Y \text{ or } Z) \) of bare paper and full-tone ink is represented by \( T_{\text{paper}} \) and \( T_{\text{ink}} \), respectively, and \( p \) is an exponent, then the proposed equations are:

\[ T_{\text{pap}}(a) = (T_{\text{paper}} - T_{\text{limit}})(1 - a)^p + T_{\text{limit}} \]  \hspace{1cm} (44)

\[ T_{\text{dot}}(a) = T_{\text{limit}} - (T_{\text{limit}} - T_{\text{ink}}) a^p \]  \hspace{1cm} (45)

where, \( T_{\text{pap}} \) and \( T_{\text{dot}} \) represent the TSV of the unprinted paper inside the ink dots and of the ink dots, respectively, for any arbitrary ink coverage, \( a \). The MD model was modified to incorporate these changes in order to calculate the average tint \( \hat{T} \) of the halftone image as follows:

\[ \hat{T}(a) = aT_{\text{dot}}(a) + (1 - a)T_{\text{pap}}(a) \]  \hspace{1cm} (46)
The accuracy of Equation 46 depends on the exponent $p$ that is fitted into the measured data. It is mentioned that $p$ captures the light scattering effect as a function of the paper spread function, dot geometry, and screen frequency. The same study [38] was also based on the assumption of the uniform thickness of ink dots, and the results were based on halftone prints with low screen frequency. Furthermore, $T\text{limit}$ was theoretically calculated.

Assume $n$ is the total number of single ink separation ramps, $T$ denotes measured tristimulus value ($X, Y$ or $Z$) and $\hat{T}$ denotes corresponding tristimulus value calculated according to Equations 44-46. One thus seeks the value for $p$ which minimizes the deviation between predicted $\hat{T}$ and measured $T$, by quantifying the sum of square differences of the components [85],

$$\arg \min_p \frac{1}{n} \sum_{i=1}^{n} \left( \sqrt{(\hat{T}_i(p, a_i) - T_i)^2} \right) / n \quad (47)$$

Equation 47 can be calculated following an iterative approach by sequentially changing the value of $p$, or using non-linear least squares analysis. In this dissertation, non-linear least squares analysis was used to determine $p$ using Matlab® function \texttt{lsqnonlin()}.

### 3.6 BASIC COLORIMETRIC CONCEPTS

According to the trichromatic generalization [96], a color can be specified by three numbers, transforming the spectral power distributions (SPDs) of a stimulus. A color specification system or color model is used to define colors, discriminate, judge similarity or identify color categories [97]. Some colorimetric basics relevant to this dissertation are presented in this section following the studies [96, 98, 99, 100].

#### 3.6.1 Additive and subtractive color system

**Additive color mixing:** This is a technique to obtain colors by mixing three colored lights (primary colors) in different proportions. A primary color cannot be generated by mixing the other primaries. In practice, the primary colors can be considered
as the reference standards in the mixing process. A large number of colors can be generated using red, green and blue as the additive primaries. Fig. 3-28 (right) illustrates that a source of light is shown on the B side, whereas three primary colors are projected on the A side to obtain the mixed color. An observer tries to match the source color with the mixed color by changing the proportion (relative luminance) of the primary colors.

Figure 3-28: Illustrating additive color mixing process.

**Subtractive color mixing:** In the graphic arts industries, subtractive color mixing is predominantly used to obtain different colors. In this system, the mixing lights are first passed through different color filters or reflected by different pigments. Fig. 3-29a shows that we can obtain the additive primaries by mixing two subtractive primaries. Mixing all three yields black. Fig. 3-29b explains that, in contrast to additive mixtures, it is necessary here to subtract the light spectrum, which is absorbed by the pigments or filtered. The primary colors in this system are cyan, magenta and yellow.

Figure 3-29: Subtractive color mixing process: (a) Mixtures of light through filters (b) reflected by pigments.
3.6.2 Color matching experiment
Additive color mixing is the base for the development of a color mixing system. Any color can be quantitatively expressed by the amounts of primary colors required for the matching. Proportionality and additivity are the basic laws of mixtures for color matching. Mathematical notations are used to express color matchings and the basic laws.

Grassman Laws: A color is represented by \([Q]\) and when two colors match, the matching can be expressed as:

\([Q_1] = [Q_2]\)

A) Proportionality: Color matching holds when the SPDs of all the components are multiplied by a constant \(\varepsilon\).

If \([Q_1] = [Q_2]\) then \([\varepsilon Q_1] = [\varepsilon Q_2]\)

B) Additivity: Color matching holds for stimuli obtained by adding color-matched stimuli.

If \([Q_1] = [Q_2]\) and \([Q_3] = [Q_4]\) then

\([Q_1 + Q_3] = [Q_2 + Q_4]\)

Additive color matching using primary stimuli: Given the primary stimuli \([R]\), \([G]\) and \([B]\), in general, we can mathematically write the following equation for a color matched stimulus:


where the color stimulus has matched by the amounts \(R, G\) and \(B\). These \(R, G\) and \(B\) are the tristimulus values of \([R]\), \([G]\) and \([B]\). The \(R, G\) and \(B\) are the relative or normalized values of luminance. When \(R = G = B\), the stimulus matches a specified standard stimulus (equi-energetic white). That is:

\[ R = \frac{p_R}{L_R}, \quad G = \frac{p_G}{L_G}, \quad \text{and} \quad B = \frac{p_B}{L_B} \]

where \(p_R, p_G\) and \(p_B\) are the luminances of \([R]\), \([G]\) and \([B]\) in the matching, and \(L_R, L_G\) and \(L_B\) (luminous units) are the luminances of \([R]\), \([G]\) and \([B]\) for the reference white.

Let \([q_{\lambda}]\) represents a test stimulus of single wavelength(\(\lambda\)) and unit radiance. In the additive mixing process, if the stimulus is
matched by the primary stimuli, then the color matching equation can be written,

\[ q_\lambda = r_\lambda [R] + g_\lambda [G] + b_\lambda [B] \]

where \( r_\lambda, g_\lambda \) and \( b_\lambda \) are familiar as color matching coefficients.

The same color matching experiment is conducted for all the components in the visible spectrum to obtain the color matching coefficients. The set of color matching coefficients for the visible spectral range is known as the color matching functions (CMFs) for the RGB primaries.

If \([P]\) is a polychromatic stimulus with a SPD \([P_\lambda]\), the stimulus can be expressed as sum of monochromatic stimuli:

\[ [P] = \sum_{\lambda} [P_\lambda] = \sum_{\lambda} P_\lambda q_\lambda \]

According to Grassmann’s law:

\[ [P] = \sum_{\lambda} P_\lambda (r_\lambda [R] + g_\lambda [G] + b_\lambda [B]) \]

\[ = \sum_{\lambda} P_\lambda r_\lambda [R] + \sum_{\lambda} P_\lambda g_\lambda [G] + \sum_{\lambda} P_\lambda b_\lambda [B] \]

In terms of tristimulus values and the primaries, \( P \) can be expressed as:


By identifying the terms in the two expressions of \( P \), a simple formula can be derived for calculating the tristimulus values:

\[ R = \sum_{\lambda} P_\lambda r_\lambda, \quad G = \sum_{\lambda} P_\lambda g_\lambda, \quad B = \sum_{\lambda} P_\lambda b_\lambda \]

So the tristimulus values of a color can be calculated from the SPD and tabulated color matching functions. The average of color matching functions of a set of observers is used as the common functions for color matching.

3.6.3 CIE color specification systems

**RGB color system:** In 1931, the CIE established three monochromatic stimuli of wavelengths 700 nm, 546.1 nm and 435.8 nm as the \([R], [G] \) and \([B] \) standard primaries, respectively. The amount of \([R], [G] \) and \([B] \) stimuli required to match the white reference stimulus are in the ratio 72.1:1.4:1.0 [96]. The CIE adopted the average color matching functions of seven and ten
observers with normal color vision experimented by Guild and Wright in two different experiments [96]. Fig. 3-30 shows the CIE 1931 RGB color matching functions $\bar{r}(\lambda)$, $\bar{g}(\lambda)$ and $\bar{b}(\lambda)$. Notice that for some monochromatic stimuli the negative amount of red is required to obtain the tristimulus value. This is because those stimuli are very saturated and added amount of red is required to subtract to obtain the target color.

Figure 3-30: CIE 1931 RGB color matching functions.

If a spectrum $P(\lambda)$ is given, then the RGB colors are calculated by the following integrals in the visible (Vis) range:

$$R = k \int_{\text{vis}} P(\lambda) \bar{r}(\lambda)$$
$$G = k \int_{\text{vis}} P(\lambda) \bar{g}(\lambda)$$
$$B = k \int_{\text{vis}} P(\lambda) \bar{b}(\lambda)$$

The constant $k$ will be described in the following section. The vector components $(R, G, B)$ can specify any color $[P]$ in a three-dimensional space named as RGB color space. The vector $(R, G, B)$ can be normalized as follows:

$$r = R / (R + G + B)$$
$$g = G / (R + G + B)$$
$$b = B / (R + G + B)$$

The $(r, g, b)$ intersection points of the vectors $[P]$ and the plane $R + G + B = 1$ are known as chromaticity coordinates. In this unit plane any color can be located by the two coordinates out of three.
A chromaticity diagram represents the two chromaticity coordinates in this plane.

**XYZ color system:** A color specification system can be converted to a new one applying a linear transform relating the tristimulus values in both systems [96]. To avoid the negative values in RGB color matching functions, in 1931, CIE defined a new set of primaries \([X], [Y] and [Z]\) related to the original RGB set by a linear transformation. This alternative color specification system is known as the CIE 1931 XYZ color specification system. A fundamental aspect of this new system is that one of its color matching function is made equal to the luminous efficiency curve \((V_\lambda)\). This is due to express the stimulus luminance by the tristimulus value \(Y\) directly. The linear transformation [101] that rules the change of RGB and XYZ coordinates in the CIE color systems is given below.

\[
\begin{pmatrix}
\bar{x}(\lambda) \\
\bar{y}(\lambda) \\
\bar{z}(\lambda)
\end{pmatrix} =
\begin{pmatrix}
0.49 & 0.31 & 0.2 \\
0.17697 & 0.81240 & 0.01063 \\
0.0 & 0.01 & 0.99
\end{pmatrix}
\begin{pmatrix}
\bar{r}(\lambda) \\
\bar{g}(\lambda) \\
\bar{b}(\lambda)
\end{pmatrix}
\]

This transformation enables the new \(X, Y\) and \(Z\) primaries to form a triangle in the chromaticity diagram that includes all real colors inside the least area possible. These CMFs (Fig. 3-31a) are referred as the CIE 1931 2° colorimetric observer or standard observer since they were obtained for a 2° central vision field.

*Figure 3-31:* (a) The CIE 1931 XYZ color matching functions, (b) The CIE 1964 XYZ color matching functions.
Another set of CMFs were obtained experimentally for vision field of 10° by Stiles and Burch (49 observers) and Speranskaya (27 observers) [96]. The average result is known as the CIE 10° colorimetric observer or the CIE 1964 standard colorimetric observer. The CIE selected the primaries so that the CMFs for 10° standard observers (Fig. 3-31b) are not exceedingly different than CIE 1931 standard CMFs. The CIE 1964 CMFs yield some differences [102] in the color matching process due to different distributions of photoreceptors in the retina and macular pigment in the central position of visual filed. Therefore, the new CMFs are suitable for viewing fields usually larger than 4°.

### 3.6.4 Calculation of CIE tristimulus values

The general equations for calculating the CIE tristimulus values in CIE 1931 colorimetric system are [96]:

\[
X = k \int_{\lambda} P(\lambda) \bar{x}(\lambda) \, d\lambda \\
Y = k \int_{\lambda} P(\lambda) \bar{y}(\lambda) \, d\lambda \\
Z = k \int_{\lambda} P(\lambda) \bar{z}(\lambda) \, d\lambda
\]

where \( P(\lambda) \) denotes the spectral radiant power distribution of the given stimulus, \( \bar{x}(\lambda), \bar{y}(\lambda) \) and \( \bar{z}(\lambda) \) are CIE 1931 standard CMFs and the normalizing factor \( k \) is kept constant. If \( k = 683 \text{ lm/w} \) and \( P(\lambda) \) is the spectral radiance of the stimulus, then the \( Y \) tristimulus value would be the luminance of the stimulus. Because, the \( \bar{y}(\lambda) \) is set to the photopic luminous efficiency curve. This is applicable only in the CIE 1931 colorimetric system. In case of a reflecting object, the color stimulus \( P(\lambda) \) is:

\[
P(\lambda) = L(\lambda) R(\lambda)
\]

where \( R(\lambda) \) is the spectral reflectance of the object and \( L(\lambda) \) is the SPD of the illuminating source. The constant \( k \) is calculated to equate the \( Y \) tristimulus value of a perfect diffuser to 100. The \( Y \) value is then considered as the luminance factor. The integrals for the \( X, Y \) and \( Z \) then become:

\[
X = k \int_{\lambda} R(\lambda) L(\lambda) \bar{x}(\lambda) \, d\lambda
\]
G M Atiqur Rahaman: Use of Reflectance Measurements to Study Turbid Media by Imaging

\[ Y = k \int_{\lambda} R(\lambda) L(\lambda) \bar{y}(\lambda) d\lambda \]
\[ Z = k \int_{\lambda} R(\lambda) L(\lambda) \bar{z}(\lambda) d\lambda \]

and
\[ k = 100 / \int_{\lambda} L(\lambda) \bar{y}(\lambda) d\lambda \]

To replace the integration by summation the most commonly used method is the \textit{weighted-ordinate} method [96] as shown below:

\[ X = k \sum_{\lambda=\lambda_{\text{min}}}^{\lambda_{\text{max}}} R(\lambda) L(\lambda) \bar{z}(\lambda) \Delta\lambda \]
\[ Y = k \sum_{\lambda=\lambda_{\text{min}}}^{\lambda_{\text{max}}} R(\lambda) L(\lambda) \bar{y}(\lambda) \Delta\lambda \]
\[ Z = k \sum_{\lambda=\lambda_{\text{min}}}^{\lambda_{\text{max}}} R(\lambda) L(\lambda) \bar{z}(\lambda) \Delta\lambda \]

The visible spectrum \((\lambda_{\text{min}}: \lambda_{\text{max}})\) is divided into equal widths \(\Delta\lambda\) centered at wavelength \(\lambda\). The radiant power \(L(\lambda)\) at wavelength \(\lambda\) is assumed constant within the interval of width \(\Delta\lambda\) [96]. The same set of equations also apply for calculating tristimulus values in CIE 1964 colorimetric system except that the CMFs would be replaced by the CIE 1964 CMFs. Another exception is that the Y tristimulus value has no photometric significance.

### 3.6.5 CIE 1931 \((x,y)\)-chromaticity diagram

The chromaticity diagram represents the \((x,y)\)-coordinates as a parametric \(x-y\) plot [97]. The tristimulus values of any color stimulus can be converted to CIE 1931 \((x,y)\)-chromaticity coordinates by normalizing the \(X, Y, Z\) values as follows [97]:

\[ x = \frac{X}{X + Y + Z}, \quad y = \frac{Y}{X + Y + Z} \]

The chrominance components of a given color are jointly described by the \((x,y)\)-chromaticity coordinates. Fig. 3-32 shows the CIE 1931 \((x,y)\)-chromaticity diagram that represents every physically realizable color as a point.
Theory

The diagram has an inverted U-like shape. This diagram has the boundary, which is known as the spectral locus, represents the chromaticity coordinates of all the primary sources. Each end of the spectral locus is joined by a straight line known as the purple boundary. The equi-energy white point has the coordinates at \( x = y = 1/3 \). From the white point more saturated colors radiate towards the boundary. Any visible chromaticity of an additive mixture will have a corresponding point on this diagram. A straight line will pass through the point and its constituents of the mixture of two color stimuli [96]. The dominant wavelength or the hue of a color is defined as the intersection point of a line drawn from the reference white through the given color to the spectral locus. The saturation is defined as the ratio between the line segments that connect the white with the color and the white to the dominant wavelength [97]. The red and blue wavelengths are mixed to generate the colors on the purple boundary.

![Diagram](image.png)

*Figure 3-32: The CIE 1931 (x,y)-chromaticity diagram [103].*

3.7 **IMAGE SEGMENTATION METHODS**

A common consensus among researchers is that there is no one perfect solution for image segmentation. The best algorithm is the one that can provide an optimal or a generally acceptable solution for a given subject matter [104]. Selecting an algorithm is relatively important when different imaging modalities (e.g., co-registered RGB-spectral cameras) provide different levels and
types of information. The article in Ref. [104] provides an excellent review of state of the art image segmentation methods.

To physically measure the areas of solid ink, mixed areas, and the paper between the dots of a halftone print, we had to segment the microscale RGB images. The images were acquired by three different imaging modalities (section 3.3). The issue of choosing a segmentation method became simple as we looked at the gray-level image/plane that corresponds to a single primary ink (C, M or Y). Because the respective gray level images show the best contrast in intensity from the three regions. (For more details, refer to section 4.1.) This is the basis for choosing the spatially blind segmentation approach that is well known to perform in the attribute/feature space, predominantly related to intensity [104]. Clustering and histogram thresholding are the two popular techniques used in this approach.

In the first study (Paper I), we intuitively applied standard k-means clustering to segment the gray level image into the three aforementioned regions. However, the analysis of the overall results, which indicated room for further improvement, led us to apply hierarchical cluster analysis for histogram thresholding (Paper II). In a single ink halftone image, where the nominal coverage is above around 60%, the inks overlap. These images, therefore, have another region where the intensity is different from the other regions. The k-means algorithm does not take account of this issue, therefore, produced suspicious results for nominal coverage over 60%. The algorithm may also be influenced by outliers and empty clusters. In addition, the k-means algorithm can converge to local optima, leading to non-optimal solutions.

3.7.1 k-means clustering
We viewed the image data as a point cloud on a one-dimensional gray scale axis. The k-means clustering protocol analyzes the gray intensity point cloud to partition according to the given objective functions into meaningful pixel groupings known as clusters. Fig. 3-33 describes this protocol where the centroids of the k clusters are used to characterize the pixel values of an image. For the set
of data elements\((I_1, I_2, \ldots, I_N)\) in an image vector \(I\), this technique aims to segment the elements into \(k (\leq n)\) clusters \(C = \{C_1, C_2, \ldots, C_k\}\). The standard algorithm [105] assigns the data elements among the clusters to minimize the within cluster sum of the squared distances. The objective function can be represented as:

\[
\arg\min_{C} \sum_{i=1}^{k} \sum_{I \in C_i} ||I - \mu_i||^2
\]

where \(\mu_i\) is the mean of the elements in cluster \(C_i\).

Fig. 3-33: Illustration of k-means clustering process: (a) initialization of means (b) assignment of each element to the nearest mean (c) re-estimate means

Fig. 3-33a describes the clustering process in case of 3-means. At first (Fig. 3-33a) three random points are assigned to the means of three clusters. In the next step, distance between each point and each mean is determined. The point closest to the mean is assigned to the respective cluster of that mean (Fig. 3-33b). The mean of each cluster is re-estimated (Fig. 3-33c) and the procedure repeats until there is no change in clustering assignments. The following algorithm was used to apply k-means clustering in the study.

---

**Iterative approach to implement k-means clustering**

1. Choose \(k\) data elements at random to set them as the \(k\) initial cluster centers (centroids): \(c_1, c_2, \ldots, c_k\). (Fig. 3-33a)
2. Compute the distances from all the data elements to each of the cluster centroids as:

\[
d_{i,j} = \left(\|c_i - I_j\|\right)^2, \quad i \in \{1,2, \ldots, k\}, j \in \{1,2, \ldots, N\}
\]
3. Assign each data element \( I_j \) to the cluster \( C_i \) corresponding to the minimum distance of \( d_{i,j} \). (Fig. 3-33b)

4. Compute the arithmetic mean of the elements in each cluster \( C_i \) in order to obtain \( k \) new centroid locations. (Fig. 3-33c)

5. Repeat steps 2 to 5 until the cluster assignments do not change or the maximum number of iterations is reached.

Since arithmetic mean is a least-squares estimator, this algorithm minimizes the within cluster sum of the squared distances.

### 3.7.2 Hierarchical cluster analysis

The histograms of grayscale halftone images are of different modalities due to being functions of the nominal ink coverage. Hence, the selection of the proper thresholds is the key to accurate segmentation and thus to the parameter estimation of halftone reflection models [65, 66]. The segmentation method adopted in the study of Paper II was based on a hierarchical cluster analysis. The original idea was first proposed for determining a single threshold from a grayscale image [106]. In this study, the idea has been applied to determine two optimal thresholds so as to segment the image into three regions.

The threshold selection technique is illustrated in Fig. 3-34 for \( k=3 \) (i.e. \( k-1=2 \) thresholds). Assume that the gray level values are organized in ascending order. Note that, in practice (Paper II) the means and variances of the clusters and the cluster after the possible merging operation are used for the distance measurement [106]. Here, for illustrating the operations in Fig. 3-34, we use Euclidean distance metric, and the highest value in a merged cluster as the cluster representative. The technique begins assuming that each non-empty gray level of an image histogram is a cluster. Then, the clusters with the closest distances (red colored number in Fig. 3-34) are merged in the next level, and the highest value is set as the class representative. The process continues until we have \( k \) clusters. The first \( (k-1) \) values are the desired thresholds in the remaining \( k \) number of clusters.
Figure 3-34: Illustration of hierarchical cluster analysis for image segmentation.

Assume that $C_n$ is the $n$-th cluster of gray levels, while $I_n$ is the highest value in $C_n$. Additionally, assume that $C_n$ is organized in ascending order. The mathematical formula for distance calculation is available in [106]. The algorithm [106] for merging the clusters in order to determine the thresholds is described below.

---

**Determine multiple thresholds from image histogram**

1. Assign each cluster $\{C_1, C_2, \ldots, C_n\}$ to each of the non-empty gray levels $\{I_1, I_2, \ldots, I_n\}$ of the image histogram.
2. Compute the distance $d_i, i \in \{1, 2, \ldots, n-1\}$ between every pair of adjacent clusters.
3. Find the smallest value of $d_i$ and unify this pair of clusters into one cluster.
4. Update the index of clusters to $\{C_1, C_2, \ldots, C_{n-1}\}$. Similarly, update the index and values of $\{I_1, I_2, \ldots, I_{n-1}\}$.
5. Repeat steps 2 to 4 $(n-k)$ times where $k$ is the number of target clusters.
6. The final set of clusters is $\{C_1, C_2, \ldots, C_k\}$ and $\{I_1, I_2, \ldots, I_k\}$ represents the highest gray levels, respectively.
7. Output $\{I_1, I_2, \ldots, I_{k-1}\}$ as the estimated thresholds.
3.8 SPECTRAL BAND SELECTION TECHNIQUE

Scattering and absorption occur when electromagnetic waves interact with dyed fibers. The nature of the molecular bonds primarily influence the region of the spectrum where the absorption takes place [30]. It is of great interest that strong absorption occurs between 1000nm and 2500nm when the electromagnetic waves interact with the natural fibers [30]. The peaks appear where the vibrations in the electric field of a dipole dominate by absorbing energy from the radiation.

Wavelength bands in a wider spectral range may have features that can be used to identify the dyes [30, 107]. The focus of the study (paper III) was to develop a deterministic approach using spectral reflectance to classify the fiber dyes into natural or synthetic class. The major motivation of the study was to show that diffuse reflectance has the potential to leverage information in manifesting dye identity.

In this study (Paper III), we applied the sparse logistic regression technique with a Bayesian regularization to identify the spectral bands in order to classify fiber dyes. In the literature [108], this regression model was generally recommended to eliminate insignificant features and retain the most relevant features for the class separation. Although the technique was originally proposed for gene selection in cancer classifications [108, 109], it has recently been used successfully in band selection for spectral data classifications [110, 111, 112]. In our study, the same algorithm [113] also showed effective in selecting the discriminative wavelength bands.

3.8.1 Bayesian probability

Bayesian probability theory is a mathematical framework that uses probability for inference or reasoning. In the case of noisy, sparse or uncertain data, the framework is most often used to justify the relative validity of a hypothesis. It is also used to adjust the parameters of a specific model [105]. If A and B are two events, the joint probability can be expressed as:

\[ P(A, B) = P(A|B) P(B) = P(B|A) P(A) \]
In other words, Bayes’ rule just involves manipulation of the conditional probabilities. In this theory, one of the events is the hypothesis \( C \), and the other is data \( x \). Bayes’ rule estimates the relative truth of the hypothesis as follows,

\[
P(C|x) = \frac{P(x|C) P(C)}{P(x)}
\]  

(49)

Here, \( P(x|C) \) is known as the likelihood function that assesses the probability of the given data \( x \) arising from \( C \). The term \( P(C) \) (known as prior) represents one’s prior knowledge before the data are considered. The term \( P(x) \) is obtained as follows,

\[
P(x) = \sum_C P(x|C) P(C)
\]  

(50)

Since \( P(C|x) \) represents the probability of the hypothesis after considering the data, the term is known as posterior.

### 3.8.2 Regression analysis

In regression, some functional description of data is sought mostly with the aim to predict values for new input [105]. Suppose, we have a vector of inputs \( x = (x_1, x_2, \ldots, x_n) \) and corresponding vector \( y = (y_1, y_2, \ldots, y_n) \). Then for example, in linear regression, the function \( E(y|x) \) is linear in the input variables \( x_1, x_2, \ldots, x_n \). The linear regression model can be written as follows:

\[
f(x) = \sum_{j=1}^{m} x_j \alpha_j + \alpha_0
\]  

(51)

In practice, we need to estimate the parameters \( \alpha \) from the given set of training data \( (x_1, y_1), \ldots, (x_m, y_m) \). Each \( x_i \) is a vector of measured features for \( i \)-th case. In least squares estimation method, the coefficients \( \alpha = (\alpha_0, \alpha_1, \ldots, \alpha_n)^t \) are chosen to minimize the residual sum of squares,

\[
Z_x = \sum_{i=1}^{m} (y_i - f(x_i))^2 = \sum_{i=1}^{m} (y_i - \sum_{j=1}^{m} x_j \alpha_j - \alpha_0)^2
\]  

(52)

This criterion is valid if the training observations \( (x_i, y_i) \) represent independent random draws. Even the criterion is valid if the \( y_i \)s are conditionally independent given \( x_i \) inputs.

Overfitting occurs when the model is too adhesive to the data and perhaps learns background noise during the fitting.
procedure. The *regularization* technique is used to solve the problem of overfitting so that the model remains accurate at prediction and generalization. For regularization, we penalized the loss function by adding a multiple ($\gamma$) of norm of the weight vector $\alpha$ that contains the learned parameters, as follows:

$$
\psi = Z_X + \gamma \left( \sum_{j=1}^{n} |\alpha_j| \right)
$$

This model prevents overfitting by tuning the regularization term $\gamma$, and can be used for feature selection for $L_1$ norm [108]. Cross-validation is an effective procedure for tuning the regularization term. The data is split to train the model for a particular value $\gamma$ and test it on the remaining data. By varying $\gamma$, the best value is selected in order to minimize the loss function. In addition, the weights that are least needed to optimize the adjusted $\gamma$ can be eliminated [105].

### 3.8.3 Sparse logistic regression technique

We have a two-class ($C_1, C_2$) problem as the given set of labeled training data is $X = \{x_i, y_i\}_{i=1}^{m}$, where $x_i \in \mathbb{R}^n$ is the $i$-th measurement vector and $y_i \in \{-1, +1\}$ is the associated class label. Then, the logistic regression approach estimates the a posteriori probability of class membership as:

$$
P(C_i|x_i) = \frac{1}{1 + e^{\gamma \sum_{j=1}^{n} a_j x_{ij} + a_0}}
$$

where the model parameter $\alpha = (a_0, a_1, \ldots, a_n)$ is the weight vector. That is, Equation 54 gives the conditional probability of input sample $x_i$ being in class $C_1$. Now, the problem converges to find the values of $\alpha$. If the training set $X$ is assumed to be an independent and identical (i.i.d) Bernoulli distribution, then one of the proposed solutions [108] is to minimize the negative log-likelihood function given as:

$$
Z_X = \sum_{i=1}^{m} \log \left( 1 + e^{-y_i \left( \sum_{j=1}^{n} a_j x_{ij} + a_0 \right)} \right)
$$

To render the model sparse rather than dense, a regularization term $\gamma$ is added to obtain the following training criteria:

$$
\psi = Z_X + \gamma \left( \sum_{j=1}^{n} |\alpha_j| \right)
$$
By a derivative analysis of Equation 56, it can be shown that if the sensitivity of the negative log-likelihood with respect to $\alpha_j$ falls below $\gamma$, then the value of $\alpha_j$ can be set to zero and the corresponding input feature can be eliminated [108]. However, there are two limitations to this approach to determining an appropriate value of $\gamma$: (1) the missing optimization problem, and (2) the need for lengthy cross-validation trials.

An alternative technique was proposed by Cawley and Talbot [109] to eliminate the regularization parameter by using the Bayesian interpretation to minimize Equation 55. In this case, the posterior distribution of the logistic regression coefficient $\alpha$ can be written as:

$$P(\alpha|X, \gamma) \propto P(X|\alpha)P(\alpha|\gamma)$$  \hspace{1cm} (57)

A separable Laplace distribution gives the prior over the model parameters $\alpha$ as:

$$P(\alpha|\gamma) = \prod_{i=1}^{N} \frac{1}{\gamma} \exp\{-\gamma|\alpha_i|\}$$  \hspace{1cm} (58)

where $N$ is the number of non-zero model parameters. The parameter $\gamma$ can be eliminated using an analytical approach as reported in [114] where the prior distribution over the model parameters is given by the marginalization over $\gamma$ as:

$$P(\alpha) = \int P(\alpha|\gamma)P(\gamma)d\gamma$$  \hspace{1cm} (59)

Since $\gamma$ is a scale parameter, in order to provide an appropriate ignorance prior, Cawley and Talbot [109] considered the improper Jeffrey’s prior [115], $P(\gamma) \propto 1/\gamma$, corresponding to the uniform prior over $\log \gamma$. The expression is obtained by substituting Equation 58 in Equation 59 and noting that $\gamma$ is strictly positive:

$$P(\alpha) = \left(\frac{1}{\gamma}\right)^N \int_0^{\infty} y^{N-1} \exp\{-\gamma(\sum_{j=1}^{n} a_j)\} dy$$  \hspace{1cm} (60)

Using the Gamma integral described in [116], the expression becomes:

$$P(\alpha) = -\log(p(\alpha)) \propto N \log(\sum_{j=1}^{n} a_j)$$  \hspace{1cm} (61)

Equation 61 gives a revised optimization function for the sparse logistic regression with no Bayesian regularization parameter:
Cawley and Talbot [109] differentiate Equations 56 and 62 to get:

$$\nabla \psi = \nabla Z_X + \gamma \nabla \left( \sum_{j=1}^{n} a_j \right)$$

and

$$\nabla \tilde{\psi} = \nabla Z_X + \tilde{\gamma} \nabla \left( \sum_{j=1}^{n} a_j \right)$$

where,

$$\tilde{\gamma} = \frac{1}{N} \sum_{i=1}^{n} |a_i|$$

From the gradient descent viewpoint, minimizing \( \tilde{\psi} \) effectively becomes equivalent to minimizing \( \psi \) when the regularization parameter \( \gamma \) is continuously modified by Equation 64. The details of the model and the optimization process for the regularization parameters are presented in [108, 109].

### 3.9 SPECTRAL IMAGE VISUALIZATION

The study in Paper IV was about methods to automatically visualize the spectral color inconsistencies of fibrous surfaces. Our interest was in a general visualization technique that could be applied to spectral scenes containing wavelength bands in infrared region (400-1000 nm). The literature survey revealed that existing methods are based on band selection, band weighting, band transformation, and optimization strategies [117]. However, most of these methods are application specific rather than general. We have investigated the pertinence of the first three strategies to visualize the spectral image of traditional carpets to exemplify the outputs. The results in Paper IV were reported based on band weighting and band selection techniques. The band weighting strategy using extended CIE color matching functions (CMF) was found appropriate for satisfying most of the common visualization goals that are described below. This technique has been discussed in this section. The other strategies are illustrated in section 4.5.

#### 3.9.1 General goals for spectral image visualization

Visualization of spectral images is an important processing step to spontaneously detect the region of interests and relevant...
features for a particular task [117]. To display the spectral scene on a tri-stimulus RGB display, it is essential to represent the scene by three wavelength bands. This implies that any spectral image displayed on a tri-stimulus display eventually loses information. On the other hand, any color value can be associated with multiple spectral vectors, and such metameric colors are interpreted by context, shape and other visual features. The accuracy of any spectral image visualization method thus depends on the given task. The authors in [43, 44] proposed a number of goals for a general spectral image visualization method, regardless of tasks. If the following goals are satisfied, the displayed scene can be interpreted quickly and accurately:

1. **Summarization**: The original spectral data should be summarized accurately. For this, all the wavelength bands should be processed similarly in a general sense. If necessary, specific bands can be processed to highlight any region of interest.

2. **Consistent rendering**: Any spectrum is always displayed with the same color across the images. Since this feature would produce a color-association system, different images would be possible to compare.

3. **Equal-energy white point**: Any spectrum that has same reflectances (for all bands) is displayed by the shade of gray. If the reflectance value is zero or maximum, the spectrum should be mapped to black and white of the display, respectively.

4. **Minimum pre-attentive features**: Unnecessary distractions of viewers by sudden attractive colors that are non-informative are minimized. For example, the method would not display unintentionally brightly saturated colors on a background of different color.

5. **Natural palette**: A natural palette and distribution of colors are used to be consistent with natural images [44, 117]. By attaining this goal, inaccuracies in quantitative judgement of colors between small color regions can be avoided.
6. **Wavelength shift invariance**: In any spectral range, the visualization method works equally for any number of spectral bands. In addition to spectral zooming or panning, this goal enables the method to work for a new instrument.

7. **Smallest effective difference**: The relative differences are shown no larger than needed for visual distinctions.

8. **Computational Ease**

### 3.9.2 Visualization using extended CIE CMFs

It has been shown that spectral band weighting based visualization method, using three fixed weighing functions, can achieve most of the general visualization goals [44]. The technique can be applied for any spectral range beyond visible range. The working principle is similar to image computation in the visible range, if extended CIE color matching functions (CMF) are used as the weighting functions. The exception is in using deterministic weighting instead of the probabilistic sensitivity of the cones. Several spectral weighing functions (spectral envelopes) have been proposed [44], and extended CIE CMFs are shown to be effective in general for rendering colors in the range (400-2500 nm).

A number of studies [43, 44, 118] reported success for general spectral image visualizations using standard CIE 1964 tristimulus CMFs as the spectral envelopes. In this approach, the original spectral image is linearly integrated by three spectral envelopes and the rendered images are displayed as R, G and B channels. Assume a point \((i,j)\) on the image surface has reflectance vector \(\mathbf{r} \in \mathbb{R}^{nx1}\). Let the spectral envelopes are \(\overline{x}_e, \overline{y}_e\) and \(\overline{z}_e \in \mathbb{R}^{nx1}\) which are the weights of spectral bands corresponding to red, green and blue color. The proposed visualization method calculates,

\[
\begin{bmatrix}
\text{Red} \\
\text{Green} \\
\text{Blue}
\end{bmatrix}
_{ij} =
\begin{bmatrix}
\overline{x}_e \\
\overline{y}_e \\
\overline{z}_e
\end{bmatrix}
\mathbf{r} \tag{65}
\]

The technique lies in designing \(\overline{x}_e, \overline{y}_e\) and \(\overline{z}_e\) in such a way that mimics most of the aspects relevant to natural image processing.
within visible range. For example, the goal *computational ease* is achieved by fixing the weighs of the spectral envelopes, the goal *equal-energy white point* is achieved by making the total weight of each envelope equal as shown below, and so on.

$$\sum_{n=1}^{N} \bar{x}_e[\lambda_n] = \sum_{n=1}^{N} \bar{y}_e[\lambda_n] = \sum_{n=1}^{N} \bar{z}_e[\lambda_n]$$

The *wavelength shift invariance* goal was achieved by interpolating the standard CMFs for the desired spectral range beyond the visible range.

In this technique, the standard CMFs are first transformed to the sRGB color space, and multiplied by D65 illumination. The wavelength scale is then stretched to cover the target spectral range. Fig. 3-35 displays the spectral envelopes stretched up to 1000 nm. To perform the stretching operation, the first valid band of the spectral image was equated to 400 nm, whereas the last valid band was equated to 680 nm. Thereafter, a linear interpolation was applied for the values of the bands between them. The figure shows that one of the envelopes (red) has negative values, which were obtained due to the limited color gamut of the display device. If there are any negative sRGB values after integration with the original spectral image, these values are set to 0 or 255.

![Figure 3-35: Spectral envelopes ($\bar{x}_e(\lambda)$, $\bar{y}_e(\lambda)$ and $\bar{z}_e(\lambda)$) generated by adopting the CIE 1964 CMFs. The CMFs are first transformed to sRGB color space, multiplied by D65 illumination and then stretched across desired wavelengths.](image-url)
This set of spectral envelopes also ensures the important goal of **consistent rendering**. There are other possibilities of design choices like piecewise linear [44], constant-luma disc basis, unwrapped cosine basis [43] etc. But, the CIE CMFs based envelopes (Paper IV) generated the best result satisfying well most of the goals for the given set of spectral images of carpets in the range (400-1000 nm).
4 Experimental Studies and Results

4.1 HALFTONE PRINT ANALYSIS BY MEANS OF A NOVEL STRATEGY

In halftone prints, the physical interaction between the ink and paper causes for physical/mechanical dot gain [36], while the effect of light scattering appears as optical dot gain [81]. The ultimate consequence is a change in dot area and color from what was intended. Therefore, effectively incorporating this change is crucial to the accuracy of the color prediction model (CPM). In the first part of the study detailed in Paper I, the dot gain was measured by microscale image analysis (MIA) and then compared to the conventional estimation technique (in practice) using the Murray-Davies (MD) reflection model [76]. The classic MD model parameters are defined as the fractional area coverage of the dots and the unprinted paper between the dots. It is assumed that the print has dots of uniform thickness.

In this study, a novel strategy was used to analyze the microscale images of halftone prints. The aim was to better account for the light reflected off the surface that was examined in the second part of Paper I. Microscopic investigation illustrated that the dot area had variable densities, especially around the edge due to ink spreading, penetration, and lateral light scattering (Fig. 4-1a). In this context, the area of an ink dot was treated as consisting of two parts: a solid and a mixed area. Therefore, it was possible to identify those areas by the intensity variations of reflected light. This is illustrated in Fig. 4-1b, which shows that the signals going to the observer from different halftone areas are of different intensities. Obviously, the highest intensity comes from the paper between the dots (arrow ‘a3’),
while the lowest comes from the solid part of the ink (arrow ‘a1’). According to the signal processing viewpoint, the ink dots and unprinted paper can be considered to be the main sources of the signals. The local variations in the paper surface should be treated as noises, although the signal distortions in the mixed areas should be separately measured and characterized.

Figure 4-1: Schematic diagram of halftone prints: (a) dot area fragments, and (b) source of signals to the sensor [37].

Based on the above hypothesis, each digital image was considered to be a measurement of the reflected light affecting either the N-bit brightness value (in a gray level image) or the trichromatic color vectors (in an RGB image). Thus, the signal captured by the imaging sensor was able to differentiate between the sources. To verify this notion and observe the results on media variations, samples were prepared using variations of inks, papers, halftone method, and printing technology. The microscopic imaging set-up described in section 3.3 was used to acquire the RGB images of the print samples. Fig. 4-2a shows average gray level profile of 50% Cyan coverage on offset (AM) print, and Fig. 4-2b highlights the profile covering entire area of a random dot.

Figure 4-2: (a) Horizontal average gray level profile of 50% Cyan offset (AM) image, (b) intensity profile spatially covering a complete dot
A simple \textit{k-means} clustering algorithm was applied to segment the gray level image of a microscale halftone print. At the beginning of the process, the number of clusters was set to a maximum of three. The clusters with lowest, middle and highest mean values were defined as of solid ink, mixed area and paper, respectively. Fig. 4-3a depicts the gray level distribution of a line scanned across an ink dot in the image of 50% cyan (AM) offset print. Fig. 4-3b shows the gray level distribution of the solid ink area that was segmented by clustering technique. The range of the values is from 0.2 to 0.4. However, the mixed area (Fig. 4-4a) is characterized by a steady decrease or increase of values, depending on the direction. Therefore, the value is higher if the point is closer to the unprinted paper. In addition, the length of the mixed area is identical (10 pixels wide) on both sides of the dot, indicating that this is a commonly occurring phenomenon.

Let $\sigma$ be the overall standard deviation of the gray level image, and let $\theta$ represent a threshold value. After associating the intensity variations roughly with a Gaussian distribution [76], and after analyzing the FWHM of the distributions empirically, the following relation was found:

$$0 < \theta_{\text{solid}} \leq 2.9\sigma < \theta_{\text{mix}} \leq 4.5\sigma < \theta_{\text{paper}} \leq 1$$
Instead of applying the clustering technique, the derived thresholds can be used to segment the image by tuning the boundary parameters. However, note that the results reported in this thesis (Paper I-II) are based on image segmentation using the clustering approach. This is because the total dot gain characterization curves, obtained by the clustering technique, were in accordance with the estimated curves using standard MD formula (Fig. 7 in Paper I).

Figure 4-4: Pixel value distribution in a segmented image: (a) mixed area (b) unprinted paper [37]

The method and formulas described in Paper I were used to process the image and calculate the fractional area coverage of the solid ink, mixed area, and paper between the dots. As examples, Fig. 4-5 (a-d) shows, sequentially, the input image (50% cyan), separated unprinted paper between the dots, solid ink, and mixed areas that appear as shades of the solid inks. The sample in the first row comes from offset printing with FM halftoning on semi-gloss paper, while in the second row, the sample comes from electro-ink technology halftoned by AM on uncoated paper.
Figure 4-5: Segmented areas of 50% cyan image: (top) offset prints on glossy paper, and (bottom) electro-ink prints on uncoated paper (a: original image, b: unprinted paper, c: solid ink area, d: mixed area) [119].

Table 3 shows the calculated fractional coverage for 25%, 50%, and 75% nominal coverage of cyan ink in offset prints. In each case, FM produced a comparatively greater effective area (i.e., the overall physical dot gain) due to the larger dot perimeters. Additionally, the results showed that the area fractions were functions of the paper type.

Table 3: Calculated area fractions of offset prints (cyan ink).

<table>
<thead>
<tr>
<th>Area type</th>
<th>AM Nominal coverage</th>
<th>FM Nominal coverage</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>.25</td>
<td>.50</td>
</tr>
<tr>
<td>Solid ink</td>
<td>0.26</td>
<td>0.50</td>
</tr>
<tr>
<td>Mixed</td>
<td>0.12</td>
<td>0.18</td>
</tr>
<tr>
<td>Unprinted paper</td>
<td>0.62</td>
<td>0.32</td>
</tr>
<tr>
<td>Effective</td>
<td>0.38</td>
<td>0.68</td>
</tr>
</tbody>
</table>

Fig. 4-6 illustrates the results of the measured effective area for the three primary inks in offset prints halftoned with the FM method. Note that the cyan colorant always exhibited a higher dot gain than the magenta and yellow colorants. Fig. 4-6b shows the measured mixed area fractions as a function of the nominal coverage, while Fig. 4-6c exhibits the measured area fractions for solid ink and paper for each colorant. It is important to remember that the physical and optical dot gain cannot be separated from the total dot gain estimated by the conventional technique using the MD formula.
Fig. 4-7 shows an example comparing the reflectance prediction accuracy of the base MD model incorporating the estimated and measured effective coverage for offset (FM) prints. Note that the prediction accuracy using the measured coverage overlaps with the estimated coverage in the highly saturated regions (nominal coverage > 60%), although it is largely deviated for the lighter colors. Likewise, the magenta and yellow inks showed the same general trend in this study. This observation indicated that the MD model itself should be corrected in order to improve the accuracy. The proposed correction and its accuracy are described in section 4.2.

**4.2 PROPOSED REFLECTANCE MODEL**

The basic MD formula linearly combines the reflectance of fulltone ink and paper in order to predict the overall reflectance of a halftone print. The formula uses the fractional area coverage
as the scaling coefficient that linearly interpolates the corresponding reflectance. The fundamental assumption is that the reflectance values are constant. However, the experiments in this thesis demonstrated that not only the fractional area coverage but also the reflectance of the ink and paper vary as a function of the reference/nominal ink coverage.

In Paper I, based on this observation, an expansion of the MD formula was proposed. The basic principle was to separately incorporate the effect of the three sub-areas: solid ink, mixed area, and unprinted paper between the dots. It was still assumed that the reflectance of these areas was constant. So, the proposed formula aimed to linearly account for the additional contribution from the mixed area to the overall reflectance of the patch. The formula containing the additional term to add the scaled reflectance of the mixed area can be given as:

$$\hat{r}_\lambda(a) = a_I(a) r_{\lambda,I} + a_P(a) r_{\lambda,P} + a_{mix}(a) r_{\lambda,mix}$$  \hspace{1cm} (66)$$

where $\hat{r}_\lambda$ is the predicted spectral reflectance, $r_{\lambda,P}$ is the reflectance of paper white, $r_{\lambda,I}$ is the spectral reflectance of the fulltone ink area coverage, $r_{\lambda,mix}$ is the spectral reflectance of the mixed area, and $a_I$, $a_I$, $a_P$, and $a_{mix}$ are the fractional areas of nominal ink, solid ink, paper between the dots, and the mixed area, respectively. Obviously, the summation of the fractional coverages $a_I$, $a_{mix}$, and $a_P$ is equal to unity since they are functions of the nominal coverage, $a$.

The calculated reflectance ($\hat{r}_\lambda$) is partially corrected by the first two terms on the right-hand side due to using the more accurate fractional coverage of fulltone ink and paper. Here, the more significant aspect is the newly added (third) term that accounts for the contribution from the mixed area to the final reflectance.

To evaluate Equation 66, all the parameters related to the fractional coverage were directly measured by MIA as described in section 4.1. A conventional Gretag Machbeth Spectrolino spectrophotometer with a UV filter was used to measure the reflectance spectra of the fulltone ink and the paper. The measurement geometry was $45^\circ/0^\circ$ with D50 illumination. However, since it was not possible to measure the reference
spectral reflectance \( r_{mix} \) of the mixed area, the modeling was performed by rearranging Equation 66 as:

\[
r_{\lambda, mix} = \frac{r_{\lambda}(a)-a_l(a) r_{\lambda,l}-a_p(a) r_{\lambda,p}}{a_{mix}(a)}
\]

Equation 67 can, therefore, be interpreted as a basis for separating \( r_{mix} \) from the mean reflectance of fulltone ink \( r_{\lambda,l} \) and paper white \( r_{\lambda,p} \). Please note that due to the unavailability of spectral reflectance of the microscale image, we considered Equation 68 as an ad-hoc solution, using macroscopically measured reflectance. Therefore, as long as the ultimate result (i.e., the predicted overall halftone reflectance \( \hat{r}_\lambda(a) \)) has a reasonable match with the measured reflectance, the interpretation of \( r_{\lambda,mix} \) is not vital. This kind of ad-hoc solution was adopted in [87] to extend the MD model, where the calculated reflectance of ink and paper differs substantially [87, 88] from actual data [88], but the overall halftone reflectance matches reasonably.

The example presented in Fig. 4-8 shows the calculated spectrum of the mixed area \( r_{\lambda,mix} \), the measured spectra for fulltone cyan, and paper white. Notice that \( r_{\lambda,mix} \) has negative values in the higher absorption bands. These might occur due to inaccuracy in calculating the fractional area. The negative values could thus be avoided by scaling or optimizing the fractional area calculations. Nevertheless, the prediction accuracy of the proposed model was evaluated by incorporating \( r_{\lambda,mix} \) as obtained by straightforward calculation of Equation 68.

The proposed model (Equation 66) was used to predict the overall spectral reflectance of a halftone patch for arbitrary nominal coverages using the reference spectra shown in Figure 4-8. The predicted spectra at 25% and 75% nominal coverages are shown as examples in Fig. 4-9.
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Figure 4-8: Measured reference spectra of fulltone cyan and paper, and the calculated spectrum \( r_{\lambda, \text{mix}} \) of the mixed area [119].

Notice that the predicted values of the lighter ink (25% coverage) almost equal the measured values, although the model overestimated the darker ink (75% coverage). The other two primary inks, magenta and yellow, also showed such variations as a function of almost same ink coverages. The probable reason for this is the fact that after 60% nominal coverage the ink dots start to overlap, which leads to inaccurate segmentation and thus inaccurate computations of the fractional area.

Figure 4-9: Measured and predicted spectra by the proposed model at 25% and 75% cyan coverage [119].

The basic MD formula was compared correcting the dot gain (i.e., using the measured effective coverage) and without correcting the dot gain (i.e., using the nominal coverage). The example results for cyan ink are shown in Fig. 4-10. Notice that that the proposed model goes slightly higher in terms of the
sRMS errors starting at 75% coverage. However, the average accuracy was clearly better for the proposed model.

![Figure 4-10: Predicted sRMS errors for cyan ink [119].](image)

The analysis of the sRMS errors of all the paper grades as a function of the ink robustly indicated the relatively improved accuracy of the proposed model. However, the performance was found to be different for different inks or different ink/paper combinations owing to the different dot gain behavior, which was as initially assumed. In the next study (Paper II), the spatial variations of the reflectance of ink and paper were measured and compared with values estimated by an existing model. The aim of the procedure (as described in section 4.3) was to verify the performance of the proposed model against that of the MD model incorporating the measured variations of colorimetry.

### 4.3 COLOR CHARACTERIZATION OF HALFTONE PRINTS

In Paper II, we first studied the existing techniques for the characterization of color variations in the ink and paper in halftone prints. The characterization technique was proposed by P.G. Engeldrum [38] (see section 3.5.4). We characterized the color change in the mixed area using the same formula, albeit it in a different way. Finally, our proposed model was evaluated for overall color prediction of halftone patch by incorporating the variable colorimetry. It may be worth noting that we measured the spectral reflectance microscopically for this study. However,
since the experiment in the base study in Ref. [38] was carried out using XYZ tri-stimulus values (TSVs), we also processed the results by converting reflectance into tri-stimulus values.

It was reported in [38] that paper TSVs are linear mixtures of plain paper and a limiting TSV, whereas dot TSVs are linear mixtures of fulltone ink and the same limiting TSV. The limiting TSV refers to the TSV of the paper when the dot coverage approaches 1.0 or the TSVs of the dots when the ink coverage approaches zero. It was shown that the characterization accuracy of the internal change in color of the paper and ink was dependent on an exponential parameter $p$ (to account for the optical dot gain) that was fitted to the data. The limiting value was theoretically calculated (due to instrumental limitations) to be identical to the product of the reflectance of the bare paper and the spectral transmittance of fulltone ink [38, 87]. The basic MD formula incorporated these changes in order to calculate the average color of the halftone image. Please see 3.5.4 for further details.

In Paper II, instead of simulation, directly measured limiting TSVs were used to evaluate the formula when calculating the change in color in ink and unprinted paper. Furthermore, accounting for the effect of the solid and mixed areas, the single model parameter $p$ was analyzed to explain the lateral light scattering effect. This experiment thoroughly studied the following issues:

1. Investigated the experiment conducted by P.G. Engeldrum in [38], conventionally assuming that a single ink halftone print has two components: ink and paper. The common limiting value, both for the paper and ink, was simulated as prescribed.
2. The above issue was further studied by measuring the limiting value rather than the simulated value.
3. The change in color of the paper, solid ink, and mixed area was characterized, separately, using unique limiting value.
4. In each of the above cases, the overall halftone color prediction accuracy of the proposed model was compared to that of the basic MD model.
A set of previous print samples (set 2 in Paper I) was measured by a spectral microscopic imaging system as described in section 3.3. For each colorant, the measured values were: (1) the spectral reflectance of the solid inks, mixed area, and paper between the dots, (2) the overall reflectance of the halftone tints, and (3) the RGB image under the same conditions. In order to independently obtain the limiting values of the paper and ink, a halftone print with 95% and 3% nominal ink density was measured, respectively. A hierarchical cluster analysis based segmentation was performed on the corresponding color channel in the CMYK space for each primary ink image. The segmented binary image was used as a mask to collect the reflectance from a set of spectral images for each area type. The area fractions were calculated as described in Paper I. A nonlinear least-square optimization function (lsqnonlin in MATLAB®) was applied to fit \( p \) for any particular nominal coverage \( a \) in calculating the change in the TSV of paper and ink by the Equations described in section 3.5.4.

If \( r_{\lambda, I} \) and \( r_{\lambda, P} \) are the spectral reflectance of fulltone (100%) ink and paper white, the spectral transmittance of ink \( \tau_{\lambda, I} \) can be calculated as:

\[
\tau_{\lambda, I} = \frac{r_{\lambda, I}}{r_{\lambda, P}}
\]  

(69)

According to the findings of [38], the common limiting value \( r_{\lambda, limit} \) was calculated as:

\[
r_{\lambda, limit} = \tau_{\lambda, I} \cdot r_{\lambda, P}
\]  

(70)

The reflectance spectra were converted into TSVs for D50 illumination and 1931 standard observers. The proposed extension of the MD model in this thesis (Equation 66) was formulated for TSVs of halftone image \( T_{halftone} \) as follows:

\[
T_{halftone}(a) = a_{pap}T_{Paper}(a) + a_{solid}T_{solid}(a) + a_{mix}T_{mix}(a)
\]  

(71)

where, \( T_{Paper}, T_{solid} \) and \( T_{mix} \) are the TSVs of bare paper, solid ink and mixed area, and \( a_{pap}, a_{solid} \) and \( a_{mix} \) represent respective fractional area coverages.
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Fig. 4-11 represents the measured \( xy \)-chromaticity coordinates of the cyan, magenta, and yellow inks and the paper between the inks as a function of the reference coverage. The bare paper is represented by the central convergent point that connects the fulltone inks (at the end of the lines) by means of the broken lines. The chromaticities of the paper between the ink patterns are the dots closer to the central point. The chromaticities of the fulltone inks are on the other end of the lines and they are shown as circles. The chromaticities of the halftone inks are the dots that are closer to the fulltone inks.

![Figure 4-11: CIE \( xy \)-chromaticity coordinates of the measured paper limit (circled cross), the dot limit (circled dot), and the theoretical limit (triangle) [120].](image_url)

Fig. 4-11 also shows a triangle on each line to denote the simulated limit. The measured limits are marked by a circled cross (for paper) and a circled dot (for ink) on each line. Note that except for the magenta ink, these two measured limits were, as expected, very close to each other, although they were far from the theoretically calculated limit.

Fig. 4-12 illustrates the positions in the \( xy \)-coordinates when the inked area of the image was segmented into solid ink and the mixed area. As described in Paper II, the circled crosses in Fig. 4-12 are the measured limiting TSVs of the paper (known as limit-1), while the circled squares are the measured limiting TSVs of the solid ink (known as limit-2). Notice that there are notable...
distances between limit-1 and limit-2 for each ink. It can be seen that, as assumed, most of the color coordinates of the mixed area frequently occupy the space between limit-1 and limit-2. A comparison of the positions of the solid inks and the mixed area apparently clarifies that the colors of the solid inks were less scattered and more regularly oriented in the direction of the straight line, except for some light colors of magenta, as shown in Fig. 4-12.

Figure 4-12: CIE xy-chromaticity coordinates of the solid inks (squares) and the mixed area (dots). The circled square and circled cross represent the measured limits of the inks and paper, respectively [120].

Fig. 4-13 and Fig. 4-14 show the measured and predicted CIE X (circles), Y (dots), and Z (squares) TSVs of the solid inks and mixed area on coated paper. The lines represent the predicted values. The halftone color model (Equation 66) proposed in Paper I was evaluated using the measured limits of the solid ink, mixed area, and paper. The accuracy ranged from 1.22 to 1.76, with an average of 1.53 $\Delta E_{ab}^*$. Fig. 4-15 graphically illustrates the performance of the color prediction of halftone patches.
This investigation supported the rationale behind incorporating the change in color of the media components in the formula in the way proposed in this thesis. The analysis in Paper II revealed that the mixed area has a significant impact on calculating the color of the other image components. The value of the exponent $p$ was able to explain the lateral light scattering...
effect when the mixed area was treated as a separate media component like paper and solid ink. For example, in the case of coated paper, the range of $p$ was 0.172 to 0.262 (for the paper between dots) and 5.01 to 15.06 (for the ink dots), where halftone prints are considered to have two entities, namely, the ink dots and the paper between the dots. On the other hand, when the mixed area was treated as another entity, the range of $p$ became 0.519 to 1.13 (for solid inks) and 0.024 to 0.195 (for the mixed area). A lower value of $p$ indicates less effect from light scattering. The overall average of $p$ for solid ink was 0.738 and 0.655 for coated and uncoated paper, respectively. The higher value in coated paper could be explained by the higher screen frequency (175 lpi), which indicates a greater light scattering effect than with uncoated paper (144 lpi).

4.4 SPECTRAL CLASSIFICATION OF FIBER DYES

Scattering and absorption occur when electromagnetic waves interact with the dyed fibers. The nature of the molecular bonds influence the region of the spectrum where the absorption takes place [30]. Importantly, strong absorption occurs between 1000 nm to 2500 nm for natural fibers. In addition to that, the dye molecules may have minor but characteristics infrared absorption properties in the infrared region.

The study reported in Paper III examined the use of spectral bands for categorizing applied textile dyes into two generic classes: natural and synthetic. The hypothesis was based on different spectral light absorption and scattering properties of the components. In synthetic dyes, the molecules are synthesized for the formation of a chemical structure that renders the expected hue in the visible range. However, dyes with the same hue that are in different classes may have the same reflection properties in the visible range: VIS (400–700 nm), but a difference may arise in the range: NIR (700–1000 nm) or SWIR (1000–2500 nm) [30].

Fig. 4-16 shows all the samples examined in this study. The experiment involved textile samples that were woolen yarns.
attributed to a variety of optical and physical properties. The important aspect of the sample set was diversity in terms of the hues from both classes. Depending on the origin of the samples, they were divided into two sets: Set 1 (from Iran) and Set 2 (from Finland).

Figure 4-16: Samples of woolen fibers dyed with both natural and synthetic dyes.

Figure 4-17: Measured reflectance spectra of 114 samples dyed with natural Madder (red lines) and 34 samples dyed with synthetic dyes (blue dots); (top) in the VIS/NIR range, and (bottom) in the SWIR range.
The samples were imaged using two spectral line scanning camera systems. The specifications of the cameras are described in section 3.3. More details concerning the materials and the imaging techniques are reported in Paper III. Fig. 4-17 shows the measured reflectance spectra of the samples dyed with natural Madder (red lines) and synthetic dyes (blue dotted lines). Note that the diffuse reflectance spectra in the VIS/NIR or SWIR range contain broad emissions of many molecules. Moreover, large dimension of data is also a challenge to analyze for this particular application. As a result, use of these reflectance spectra is not straightforward to detect and identify colorants of materials. We started using PCA to analyze the spectra (Fig. 4-17) of natural Madder and the synthetic red dyes.

The eigen decomposition was performed on covariance matrix of each class of spectra. Fig. 4-18 shows the first two eigenvectors of each class in both spectral ranges. The first eigen vectors in VIS/NIR range (Fig. 4-18a, solid lines) indicate smooth distributions in most spectral regions, but noticeably, the eigen vectors in SWIR range are indicating more features. In SWIR range, the first eigen vector of synthetic class (Fig. 4-18b, solid blue line), in contrast to natural class, shows two modes between 1500 nm to 2000 nm. There are other spectral differences between the dye classes in SWIR range. For example, the differences of second eigen vectors are visible at about 1300 nm and also at about 1600 nm.

Figure 4-18: First two normalized Eigen vectors in: (a) VIS/NIR range and (b) SWIR range. The red color represents natural class and blue represents synthetic class.
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The cumulative distributions of eigen values (Fig. 4-19a), demonstrate that almost 100% variation is explained by first three and five eigen vectors for natural and synthetic class, respectively, in VIS/NIR range. On the other hand, in SWIR range (Fig. 4-19b), first four and six eigenvectors explain almost 100% variations for natural and synthetic class, respectively.

PCA represents high dimensional data in a reduced and concise space by retaining most important data directions. We investigated the suitability of using PCA to distinguish the reflectance data by dye class. The experiment was performed (first on Set-1) on nine partitioned spectral regions in order to better inspect the wavelength regions. The reflectance spectrum was divided into three subsets in the VIS/NIR range (400–700 nm, 700–1000 nm, and 400–1000 nm) and six subsets in the SWIR range: (1000–1500 nm, 1500–2000 nm, 2000–2500 nm, 1000–2000 nm, 1500–2500 nm, and 1000–2500 nm). This experiment was performed splitting the dataset random 70/30 splits into training and test data.

The eigen vectors of training data were used to compute the PCs of training and test data. A simple $k$-NN classifier was applied to distinguish between the classes. The maximum accuracy was 98% with the kappa [122] value 0.96 for this family of spectra in the range (1000-1500 nm). However, when the spectra from other samples (from Set-2) were combined, the maximum accuracy was found in wide spectral range (1500-2500 nm), but the accuracy reduced to 93% with the kappa value 0.84.

Although the classification accuracy via PCA was rational for the given dataset, it was not possible to detect and analyze
specific bands that could discriminate the dye class. However, in practice, it is convenient to use a small set of bands—to develop a customized imaging system that is affordable, for example, with the potential to be applied in-situ. It is also important to find specific discriminating bands in order to detect various dye components in the same group. For example, if we want to detect whether a Madder is of Alizarin or Purpurin origin, then it is likely that very few spectral bands will show the molecular differences.

We therefore focused on statistical methods to detect the minimum number of bands necessary to classify the dye class. To this end, we experimented with several methods before choosing the sparse logistic regression technique [109]. The most important aspect of this technique is that it is sparse, meaning that only the most informative features/bands relevant to a task are kept. The performance of this technique was also optimal in terms of the number of bands and relevant classification accuracy. The details of the model and the optimization process for the regularization parameters are described in section 3.8.

The basic strategy was to scan the labeled spectra in an organized fashion in order to determine the bands that have sufficient discriminatory properties. The band selection procedure was conducted on the same nine partitioned regions of the spectra mentioned previously. A binary classification support vector machine (c-SVM) model with a polynomial kernel of order 3 was chosen as a classifier. The kernel was chosen empirically as it generally yielded the highest accuracy compared to linear or quadratic discriminant analysis. The classification accuracies were evaluated for each subset using the leave-one-out cross-validation method [109].

The evaluation procedure was first accomplished on a small set of spectra (Fig. 4-17). These spectra were measured from 114 samples that were subject to only natural Madder and 34 samples that were subject to synthetic dyes to render red hues. The purpose was twofold. First, we wanted to evaluate the suitability of the method and interpret the results. Second, since natural Madder is a frequently used colorant in artworks, we wanted to
report the classification results separately. Table 4 shows the subsets of wavelengths and the selected bands. Note that the same wavelength bands have been selected in different subsets (highlighted in Table 4) even though the spectral range was expanded to a wider region.

Table 4: Bands selected by the feature selection algorithm.

<table>
<thead>
<tr>
<th>Case</th>
<th>WL range (nm)</th>
<th>WL (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>400–700</td>
<td>580, 590, 400</td>
</tr>
<tr>
<td>2</td>
<td>700–1000</td>
<td>700</td>
</tr>
<tr>
<td>3</td>
<td>400–1000</td>
<td>580, 400, 590</td>
</tr>
<tr>
<td>4</td>
<td>1000–1500</td>
<td>1000, 1140</td>
</tr>
<tr>
<td>5</td>
<td>1500–2000</td>
<td>1500, 1660</td>
</tr>
<tr>
<td>6</td>
<td>2000–2500</td>
<td>2000</td>
</tr>
<tr>
<td>7</td>
<td>1000–2000</td>
<td>1000, 1140</td>
</tr>
<tr>
<td>8</td>
<td>1500–2500</td>
<td>1500, 1660</td>
</tr>
<tr>
<td>9</td>
<td>1000–2500</td>
<td>1000, 1140</td>
</tr>
</tbody>
</table>

Table 5: Leave-one-out classification accuracy given the selected bands.

<table>
<thead>
<tr>
<th>Case</th>
<th>Accuracy (%)</th>
<th>Cohen’s Kappa</th>
<th>Natural error (%)</th>
<th>Synthetic error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>90.5</td>
<td>0.73</td>
<td>6.1</td>
<td>20.6</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>90.5</td>
<td>0.73</td>
<td>6.1</td>
<td>20.6</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>99.3</td>
<td>0.98</td>
<td>0</td>
<td>2.9</td>
</tr>
<tr>
<td>6</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>100</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>99.3</td>
<td>0.98</td>
<td>0</td>
<td>2.9</td>
</tr>
<tr>
<td>9</td>
<td>100</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 5 presents the leave-one-out classification accuracy given the selected bands. Note that, in case 2 and case 6, only one band was selected. In these two cases, either the classification algorithm did not converge or a whole class of samples were misclassified. These cases are marked by dashes. Notice that the bands in the SWIR range (1000–2500 nm) have a notable discriminating power when compared to the VIS/NIR range (400–1000 nm). In all the cases for the SWIR range (highlighted in Table
the classification accuracy is over 99%, with a perfect kappa value of around 1.0.

The selected pair of bands (cases 4, 7 and 9) that yielded 100% accuracy comprised the 1000 nm and 1140 nm bands. Fig. 4-20 visualizes the samples’ scatterings at 1000 nm and 1140 nm. Another pair of bands at 1500 nm and 1660 nm yielded a classification accuracy over 99%, with the kappa value equal to 0.98. Fig. 4-21 shows the samples’ scatterings at 1500 nm and 1660 nm. Notice that in both illustrations the samples are clearly separated from one another. These two illustrations thus support the resultant classification performances.

![Figure 4-20: Samples’ scatterings at the 1000 nm and 1140 nm wavelengths.](image)

![Figure 4-21: Samples’ scatterings at the 1500 nm and 1660 nm wavelengths.](image)

As the preliminary results appeared promising, the same technique was applied on the entire set of spectra combining all the samples from Set-1 and Set-2. The maximum accuracy was over 97%, with a very high confidence level. We conducted another experiment by calculating two normalized indexes using
the reflectance value of three bands. The indexes were used as features for the classification. The bands at 1640 nm, 2330 nm, and 1480 nm showed a 90.1% classification accuracy obtained by applying SVM with a simple quadratic kernel. The detailed results are reported in Paper III.

4.5 SPECTRAL COLOR ANALYSIS OF CULTURAL OBJECTS

The fibrous support (e.g. paper, textiles) and the colorant (e.g. dyes, pigments) are the subject of color variations due to various processes. Therefore, evaluating the overall color change and detecting the discolored or stained area of the objects of art and historical (A&H) significance is essential in deciding strategy to prevent/reduce the degradations, restoring colors, rejuvenating colors in virtual display [17] etc. Fast and accurate visual judgments as well as physical measurements and analysis of the color inconsistencies thus should facilitate different tasks in the contexts of museum and art galleries [13] [124, 125, 126]. Furthermore, it is of paramount interest to detect the areas of possible future color deteriorations [13]. However, in practice, this task is accomplished through visual inspection by the experts [13]. Visual inspection is not only challenging but also often erroneous. One of the reasons for this is that the spectral variations between the original and the area of interest can be narrow within the VIS range (400‒700 nm). For the same reason, the colors rendered in the VIS range and displayed on a tristimulus device are not capable to show subtle tonal variations in an optimal way.

It is observed that the color appearance of textile surface is due to the dominance of light absorption by the dyes in the visible range. In contrast, the fibers dominate absorbing light in the infrared region. It has been reported that variations in infrared absorption can describe the physical condition of the fibers, which damage the overall tone of the original color [30, 127]. In this context, we assumed that rendering colors that manifest light absorption properties in (400-1000 nm) wavelength range, should
increase the color discrimination ability. To this end, we experimented with various methods to display spectral image of classic carpets in a standard tristimulus display. The key feature was to enhance the ability in analyzing and interpreting reflectance spectra in terms of display colors.

In this study, we investigated existing methods for displaying spectral images in a sRGB display. We reported (Paper IV) the results using extended CIE color matching functions (CMF) as the spectral weights to the reflectance bands in (400–1000 nm) wavelength range. The CMFs were chosen since the prescribed technique in [44] satisfies most of the visualization goals stated in section 3.9. In addition to that, the CMFs can serve as a global reference to render colors beyond the visible range. As a result, color variations of the same object can be consistently assessed and compared by various organizations and future researchers. Studies are available where the concept of extended CMFs has been used to develop image visualization methods [128, 129].

We mentioned previously (section 3.9) that spectral image visualization methods can be categorized into four groups: transformation, band selection, band weighting, and optimization [117]. To justify the selection of CIE CMFs as the spectral envelopes, we briefly illustrate some methods in each of the first three groups using the visualization outputs. Note that an input spectrum of all maximum values was mapped to full white for every method instance. The values outside the gamut (0–255) were mapped to either 0 or 255. Before display, each RGB image was converted to sRGB. The sample set consists of four classical carpets that were studied as textile surfaces. The carpets were of various colors, designs, and size. The reflectance of the samples was measured in the VIS/NIR (400–1000 nm) range, using the line scan (push broom) camera described in section 3.3.

**Visualization method based on transformation:** A standard and commonly used approach in this group for color display is the Principal Component (PC) Analysis [130, 131]. In this approach, usually first three PC images are calculated and mapped to RGB channels. Depending on the channel mapping the color coding
can be dissimilar. The Red, Green and Blue channels were mapped to first, second and third PC images in this work. Fig. 4-22 shows several examples of original RGB image on the left and corresponding color renderings on the right. The sample shown in Fig. 4-22a has apparent color defects and we use it for showing the defects by the subsequent methods.

Notice that the color defects were revealed by PCs as shown on Fig. 4-22b. Although these defects were not resolved in the RGB image but they exist in the original sample. However, since this method is dependent on the amount of data variance, the color interpretations change for different images. For example, the reddish tones in Fig. 4-22(a,c) corresponded to totally different hues in the renderings shown in Fig. 4-22 (b,d). Moreover, highly saturated colors appeared in some regions in Fig. 4-22f that distract the viewer preattentively. This method also suffers due to computational complexity.

Figure 4-22 (a, b, c, d, e, f): (left) Original RGB images, (right) corresponding rendered images by first three PCs.
Visualization method based on band selection: In this approach, the spectrum was first divided into three subgroups (810-970 nm), (620-800 nm) and (430-610 nm) to correspond to Red, Green and Blue channel, respectively. From each group, a band was selected based on ranked coefficients. Fig. 4-23 shows the renderings (of the sample shown in Fig. 4-22a) by the bands selected according to ranked correlation coefficients and entropy. The details of the methods are available in [132]. Note that as we always include a band of infrared range, the rendered images show the color variations. However, these methods are also data dependent and thus suffer from inconsistent color interpretations across the samples. In addition to unnatural appearance, the edges e.g. in Fig. 4-23a are not strong enough for fast visual processing.

![Image renderings by the bands selected by ranked coefficients calculated using: (a) correlation (c) entropy.](image)

Visualization method based on band weighting: In this strategy, the contribution of each band is used to encode a color. The resultant image is a linear fusion of the spectral band images. The weighting functions can be fixed or they can be estimated based on pixel or input band measurements. We adopted the technique that uses fixed weighing functions (spectral envelopes) to report the results in paper IV. Extended CIE CMFs were used as the weighting envelopes on which the spectral data were projected [44].

There are other possibilities to design the basis functions such as piecewise linear, constant-luma disc, unwrapped cosine [43] etc. For illustration, Fig. 4-24 shows two examples of basis function and corresponding renderings. Note that both set of basis functions meet the general visualization goals like consistent rendering or equal energy white point but, the difference in correlating the color
to the spectrum is remarkable. For example, reddish tone in Fig. 4-24b is the indication that the spectrum is strong toward the infrared part and so on.

Figure 4-24 (a b, c d): Spectral weighting functions transformed into sRGB space and respective outputs: (top) extended 1964 CMFs, (bottom) sinusoidal cosine basis

Fig. 4-25 shows extended CMFs renderings of three carpets. Fig. 4-25a shows the conventional RGB image wherein any tonal variation is barely visible. The variations can be readily extracted in the rendering in Fig. 4-25b. Also, notice that, for example, the reddish tones in Fig. 4-25(a,c,e) are represented with the same hues in the renderings as shown in Fig. 4-25 (b,d,e). That is, the similar reflectance spectrum is represented in the rendering consistently by the same color all over the image, and looking more natural than other instances of renderings. Thereby, this strategy of rendering satisfies the goal of natural palette. It can also be noticed that the relative contrast among the neighboring areas and change of hues are more natural relative to other methods.

In Fig. 4-26, the solid arrow indicates the normal region of red hue, while the broken arrow indicates part of the region with tonal variations. The difference of up to 700 nm rendered in the conventional RGB image is not visible. However, the CIE $L^*a^*b^*$ color difference ($\Delta E$) between the normal and abnormal regions was 2.16 in the conventional RGB image, whereas the value was
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![Images of renderings by extended CMFs](image)

Figure 4-25(a, b, c, d, e, f): Illustrations of renderings by extended CMFs: (left) RGB image (right) rendering of corresponding spectral image

Figure 4-26: Illustrations with reflectance spectra from two regions that have very similar colors in the conventional RGB image, but appear different in the extended RGB image with VIS/NIR bands.

20.83 in the rendered image. The CIE $L^*a^*b^*$ values were calculated from RGB values obtained by rendering the spectra in

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(400-1000 nm) range. The Michelson’s contrast between the RGB values of the indicated areas was 0.01 in the conventional RGB image and 0.14 in the rendered image. Furthermore, the average Euclidean distance between the RGB values of the corresponding areas was 0.02 and 0.23, respectively.

We observed in this study that the visible band reflectances are dominated by the colorant molecules, whereas the NIR bands are mostly influenced the fibers. Therefore, the rendered color values are joint contributions from the colorants and the fibers. Hence, this approach could be beneficial for multiple purposes in cultural heritage applications, especially in the study of paintings for monitoring color changes or planning restoration works [13]. This assertion is supported by the fact that the images rendered by all the methods show relatively high color contrasts among the image elements when infrared information is accounted.
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5 Discussion and Conclusion

The main claims contained in the thesis are that spectral reflectance information can be used: (1) for advanced characterization of color printer, (2) for the classification of textile dyes into generic types and (3) for spectral color defect detection of textile surfaces. Paper I and Paper II support the first claim, Paper III supports the second claim and Paper IV supports the third claim.

In Paper I, the Murray-Davies reflectance formula was selected for study because the formula is the basis for many successful color prediction models (CPM) used in modern printing systems [84]. This study has demonstrated that although the physical principle behind the MD model is correct, inaccuracy stems from the complex interactions between the ink, paper, and light. A correction was applied by incorporating the experimentally measured parameters to more accurately account for the reflected light. The parameters were determined according to a new scheme that segments the printed surface into solid ink, ink/paper mixed area, and the unprinted paper between the dots. The prediction performance was consistently improved over the MD model with and without dot gain compensation, while retaining the physical plausibility of the model.

The results can be used, in addition to printer characterization, as an analytical tool for characterizing ink or paper in the graphic arts industry. Another application could be found in the paper manufacturing industry where the influence of the paper materials/processes could be finely tuned in order to achieve optimal product quality.

Note that due to the lacking of microscopic spectral measurement device, the proposed formula was rearranged to estimate the characteristic reflectance spectrum of the mixed area, using conventionally (macroscopic) measured spectra of 50% ink coverage. Although the magnitude was small, the proposed formula for halftone tint prediction degraded the accuracy for
fractional ink coverage over 70%. One possible reason for this was that in such a highly saturated density of ink dots, the dots overlap and thus induce inaccuracy into the classification of the solid ink and mixed area. Furthermore, the lateral light scattering effects could be significantly different, because less unprinted paper areas are left relative to the lower ink coverages. Therefore, the calculated reflectance of the mixed area might not be fully representative of the high-density prints. In addition, the cross-sectional analysis of a line profile shows that the reflectance in the mixed area is always transitional which should be modeled and incorporated in the formula.

Observation shows that the spectral deviation is high between measured and predicted reflectance spectra in the range 400-550 nm. In this study, we used a UV filter to measure the macroscopic spectral reflectance, but we did not use the filter while capturing the RGB images of the prints. This may also be a partial source of errors, since most commercial printing papers contain fluorescence whitening agents (FWA) [45] that can affect the color variations (and thus image segmentation) as a function of the reference ink coverage. Instead of using the sRGB (for sample set-2) image format, processing and analyzing images in the RAW format should provide results that are more accurate.

The first claim in this thesis was finally settled and reconfirmed in Paper II. The main limitation of the previous study (Paper I) was resolved by means of microscopic spectral imaging. The reflectance formula proposed in Paper I was rigorously examined, with the spectral reflectance of the halftone components (ink, paper) measured directly at each point of the print surface. Engeldrum’s model [38] was addressed in order to account for the color changes in the dots and paper. It may be worth reminding that Engeldrum’s model was centered on a limiting color value and an empirical parameter ‘p’.

In this study, it was revealed that the measured limiting value was different from the one calculated using Engeldrum’s formula. Furthermore, it was shown that instead of a single limiting value, individual limits for the paper and dots should improve the modeling of the color changes in the print
components. The analysis showed that the parameter ‘p’ not only manifests the light scattering [38], but also includes the effect of physical dot gain. Note that Arney et al. [133] introduced two empirical parameters to account for the color change in ink and paper. Although the extended MD model proposed in that study works reasonably well for overall halftone tint prediction, the modeled reflectances of the ink and paper become significantly different from the original values. In contrast, our study showed a correlation between the measured and calculated colors of paper and inks due to accounting the mixed area.

The overall color prediction accuracy of a halftone image by the proposed formula (Paper I) outperformed the MD formula in every case, even incorporating the effects of internal color changes in the ink and paper. Therefore, the study in Paper II supports the concept of segmenting the ink area into solid and mixed areas, and the means of incorporating their effects into the model. To the best of the author’s knowledge, this was the first attempt to study and improve the MD model via the segmentation of the printed image. Testing these concepts for multicolor halftone images and rendering them practically useful requires a simple method based on conventionally measured macroscopic reflectance. This study can contribute to advanced printer characterization where the influence of the ink, paper, halftone, or printing technique needs to be more precisely determined.

The third claim of this thesis was addressed in the study reported in Paper III. The primary goal of the study was to determine a small number of spectral bands in order to distinguish between the natural and synthetic dyes applied to textiles. It is known that scattering and absorption occur when electromagnetic waves interact with the blended fiber/dye components. The region of the spectrum where the characteristic absorption takes place is determined by the nature of the atoms and the bond between them [30]. Paper III shows that by computational method it possible to detect the bands that are distinctive between dye classes. A logistic regression-based feature selection algorithm was found to be effective in selecting
the most discriminative spectral bands. The analysis of the natural Madder and red color synthetic dyes revealed narrow regions in SWIR(1000-2500nm) range where clear difference in absorption of radiation happens. The adopted approach in this study thus opens opportunities for many other non-destructive investigations such as identifying subclass/component of natural dyes, identifying origin of natural dyes, quantifying dye concentrations etc.

To the best of the author’s knowledge, this type of work has not previously been reported in the literatures. This work should find applications in the field of cultural heritage, where the initial screening/mapping into the natural or synthetic class of dyes applied on historical textiles may save a lot of time and costs, as well as the parts of priceless A&H objects.

The same technique can be applied to determine the wavelength bands that are best able to identify mordants and distinguish the origins of natural dyes. Moreover, the reflectance spectra can be analyzed to predict the concentration of dyes. Further investigation is required to determine the discriminative bands and evaluate the classification accuracy when considering cotton fibers dyed with the same set of dyes. Depending on the outcomes, the analysis may determine whether the synthetic dyes change the molecular structure of the fibers [134], in contrast to natural dyes. This can help to explain the reasons behind the difference in absorption bands in the SWIR region.

As for the final claim in this thesis, it was shown in Paper IV that the reflectance in the visible to near infrared (Vis/NIR) bands (400–1000 nm) can be used to visualize spectral color differences through high contrast RGB colors in a standard tristimulus display. As a result, any inconsistency in color automatically appears that can be easily detectable. We used classical carpets and kilims to show the example outputs. The R, G, and B color values rendered by the spectral band weighting method [43] showed an enhanced contrast with respect to the conventional RGB colors. The rendered images revealed color variations that were weak or almost invisible in the original samples.
Discussion and Conclusion

As the spectral weights, extended CIE color matching functions (*spectral envelopes*) were used to calculate colors that were consistent and meaningful according to the spectra. Note that it is possible to design many other spectral weight functions to encode the NIR reflectance information into RGB colors. But perhaps the extended CIE color matching function is the most reasonable choice in satisfying the general visualization goals. Consistent rendering and specific color palette can be mentioned among the other goals, for which the extended CIE color matching functions can serve as a reference set of weighting functions to be used across the time and space. These features thus allow straightforward color comparisons of A&H objects following a standard like the visible range color matching functions.

The work detailed in Paper IV can be directly applied for various purposes when studying the colors of A&H objects in the context of museums and art galleries. In particular, this approach can be effective in detecting or predicting long-term color changes, detecting any damage during transportation, documenting conservation works, and visualizing the local degradation of colors [13, 135]. Most importantly, we assume that this approach makes it possible to some extent for prediction of future color degradation. The fact behind this assumption is that the physical condition of the fiber is manifested into the reflectance thus in the rendered colors [3]. In this experiment, only a few of the collected samples had color defects; therefore, more samples with defects in multiple hues need to be examined.

Several topics can be suggested for future work. First, the proposed reflection model for halftone prints can be investigated in case of multi-ink halftone prints. Second, the study in Paper II could be extended to correct Engeldrum’s formula for modelling color in halftoned ink and paper. Importantly, procedures are necessary to ensure the practical use of the reflection model proposed in Paper I. Third, the study detailed in Paper III can be further extended to detect the spectral bands that can identify mordants, as well as the origin and components of natural dyes, or to use the reflectance spectra in predicting dye concentrations.
Fourth, the study in Paper IV can be enhanced by applying existing computer vision techniques on the RGB renderings to automatically detect, evaluate, and quantify the extent of the spectral color defects on the surfaces of A&H objects.
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The thesis explores prospects and application areas concerning the use of spectral imaging to solve various problems. In practice, spectral properties of a scene can be used for scene understanding, object recognition or material identification. The challenge is in developing computational methods to extract and analyze the physical properties encoded in the reflectance. This thesis contributes in that track addressing problems that are needed to be solved especially in cultural heritage.