An Investigation of Multispectral Imaging for the Mapping of Pigments in Paintings

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ABSTRACT

Compared with colorimetric imaging, multispectral imaging has the advantage of retrieving spectral reflectance factor of each pixel of a painting. Using this spectral information, pigment mapping is concerned with decomposing the spectrum into its constituent pigments and their relative contributions. The output of pigment mapping is a series of spatial concentration maps of the pigments comprising the painting. This approach was used to study Vincent van Gogh's *The Starry Night*. The artist's palette was approximated using ten oil pigments, selected from a large database of pigments used in oil paintings and *a priori* analytical research on one of his self portraits, executed during the same time period. The pigment mapping was based on single-constant Kubelka-Munk theory. It was found that the region of blue sky where the stars were located contained, predominantly, ultramarine blue while the swirling sky and region surrounding the moon contained, predominantly, cobalt blue. Emerald green, used in light bluish-green brushstrokes surrounding the moon, was not used to create the dark green in the cypresses. A measurement of lead white from Georges Seurat's *La Grande Jatte* was used as the white when mapping *The Starry Night*. The absorption and scattering properties of this white were replaced with a modern dispersion of lead white in linseed oil and used to simulate the painting's appearance before the natural darkening and yellowing of lead white oil paint. Pigment mapping based on spectral imaging was found to be a viable and practical approach for analyzing pigment composition, providing new insight into an artist's working method, the possibility for aiding in restorative inpainting, and lighting design.

Keywords: Spectral Imaging, Pigment Mapping, Kubelka-Munk Theory.

1. INTRODUCTION

Multispectral imaging was originally substantiated within fields such as remote sensing and geographic information systems (GIS). Recently, this technique has been applied to examine paintings analytically for conservation purposes. In similar fashion to the identification of land-use classes and the mapping of mineral abundances in remote sensing, multispectral imaging has been used to identify pigments comprising a painting and quantify their concentrations pixel-wise. After multi-year development, the spectral accuracy of multispectral imaging is sufficient for pigment mapping, which is concerned with decomposing the spectrum of each pixel into its constituent pigments and their relative contributions. The output of pigment mapping is a series of spatial concentration maps of the pigments comprising the painting. With these pigment maps, the change of color appearance can be simulated when the optical properties of some pigments are replaced with those of the other pigments. Also, pigment composition will be beneficial for enriching the historical knowledge of the painting and will aid conservators in determining the best course for inpainting damaged areas of the painting when metamerism is an issue.

Sufficient spectral accuracy of multispectral imaging is a major requirement for pigment mapping. Multispectral imaging has been well developed over the past ten years.[1,2] A multi-year research program has been carried out at the Munsell Color Science Laboratory to build multispectral imaging acquisition systems and to test spectral reconstruction algorithms.[3] A practical spectral imaging system developed recently uses a traditional Color-Filter-Array (CFA) camera coupled with two optimized filters.[4] For each target, two RGB images are taken through each filter, so there are six channels for this camera system. The spectral reconstruction method, referred to as the Matrix R method, can achieve high spectral and colorimetric accuracies for a certain combination of illuminant and observer.[5] The camera system and the reconstruction method were used in this investigation to retrieve spectral reflectance factor of each pixel of the painting.

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The main objective of this paper is to investigate pigment mapping pixel-wise based on a multispectral image of a painting. The underlining theory for pigment mapping is Kubelka-Munk (K-M) turbid-media theory,[6] which can predict the spectral reflectance factor of a specimen from the optical properties of the specimen's constituent pigments. The use of the simplified K-M theory for the opaque case is well established in practice and well described in the literature.[7-10] Practical successes have been achieved by the reduction in mathematical complexity and elimination of controlling thickness. The simple opaque assumption was made for this investigation. Furthermore, it was assumed that a single optical constant, the ratio of absorption to scattering, would have sufficient accuracy to describe a pigment's optical properties throughout its range of concentrations, both singly and in mixtures.[11]

The post-impressionist masterpiece, *The Starry Night*, painted by Vincent van Gogh in 1889, was studied extensively in this research. The unframed painting was imaged in the conservation studio of the Museum of Modern Art, New York City. Twenty spots on the painting were selected and measured with a bi-directional spectrophotometer, an X-Rite Eye-One. The sRGB representation of the painting along with the 20 measurement spots is shown in Fig. 1. These spectrophotometric measurements were very critical. They were used to preselect ten pigments to form van Gogh's palette, and to evaluate performances for both camera prediction, the use of single-constant K-M theory and pigment mapping. (Pre-selection was required because the painting's pigments have not been determined using typical analytical methods.) The output was a series of spatial concentration maps of each pigment. With these pigment maps, the color appearance of *The Starry Night* was simulated when the optical property of darkened lead white paint was replaced with that of a modern substitution. These pigment maps provided new insight into van Gogh's working method and a valuable aid for restorative inpainting.[11]

Fig. 1. Vincent van Gogh, Dutch, 1853-1890. *The Starry Night*, Saint Rémy, June 1889. Oil on canvas 29 x 36 1/4" (73.7 x 92.1 cm). The Museum of Modern Art, New York. Acquired through the Lillie P. Bliss Bequest. Digital image © 2007 The Museum of Modern Art. In situ measurements notated.

2. METHODOLOGY

2.1. Kubelka-Munk Theory

In 1931, Kubelka and Munk[6] presented a theory to predict the amount of light reflected or transmitted by a scattering and absorbing layer given the concentration of each pigment in the layer. The simplified form of K-M theory for the opaque case can be expressed in Eqs. (1) and (2), where R_∞ is reflectance factor of an opaque layer, also called reflectivity, and K and S are the absorption and scattering coefficients, respectively, of the layer.

$$R_\infty = 1 + K/S - \sqrt{(K/S)^2 + 2(K/S)} \tag{1}$$

$$\frac{K}{S} = \frac{(1 - R_\infty)^2}{2R_\infty} \tag{2}$$

Under the assumption of additivity and scalability,[12] both the absorption and scattering coefficients of a paint mixture are linearly related to the absorption and scattering coefficients of its component paints, respectively, which is referred to as two-constant K-M theory. For the special case when the scattering is dominated by white paint, the ratio between absorption and scattering coefficients K/S for a paint mixture is expressed as a linear combination of the ratios of its component paints at unit concentration $(k/s)_i$, weighted by their concentrations c_i, as shown in Eq. (3). The subscript w specifies the white paint. The summation of concentrations equals unity. Only one parameter per paint, k/s, is required instead of two parameters, k and s, so it is called single-constant K-M theory.[13]

$$\frac{K}{S} = \left(\frac{k}{s}\right)_w + \sum_i \frac{c_i}{c_w}\left(\frac{k}{s}\right)_i \tag{3}$$

Visible inspection of the painting indicated that the paint layers were opaque, justifying the use of Eq. (1). Ideally, the two-constant form would be used. However, this required a database with at minimum, a masstone and tint for each pigment. Unfortunately, many of the pigments were only prepared as tints. As a consequence, the single-constant form of K-M theory was used, Eq. (3). Fortunately, this approach had sufficient accuracy when tested on the 20 in situ measurements. It is known that K-M theory does not consider the discontinuity of refractive indices between air and paint film, so measured reflectance factor was corrected using the Saunderson equations[14] ($K_1 = 0.03$ *and* $K_2 = 0.60$) before inputted into K-M theory [Eq. (2)].

2.2. Pigment Mapping for a Pixel

Depending on knowledge of the artist's working methods, historical context, and any prior analytical work, the materials comprising a painting may or may not be known. When known, pigment mapping seeks to find the right combination of these materials and their relative concentrations. This is achieved by using each material's optical properties and an appropriate mixing model, for example, K-M theory. The materials resulting in the best spectral match are assumed to comprise a given pixel. When unknown, "preprocessing" is required where a set of materials is selected leading to the best spectral matching of the painting's reflectance properties. One is choosing a subset of artist materials from a large database with known optical properties. The selection is guided by a priori knowledge. This latter approach was used for *The Starry Night*. An analytical study of one of Van Gogh's self portraits from the same time period was used principally to guide material selection.[15]

There are several approaches to selecting the specific materials and their concentrations from the subset. Since the mixing model can be described mathematically as a multivariate linear regression model, stepwise regression,[16] which automatically chooses candidate variables based on some statistical fit criterion (e.g., T statistic, partial probability, Mallow's Cp), could be used, in similar fashion to selecting pigments for inpainting.[11] However, this algorithm is highly dependent on the criteria of entering and removing that determine which variable is entered into and removed from the linear model. Also, concentrations cannot be constrained. As a result, the optimal solution may not be found. Another approach is a combinatorial approach where each combination is evaluated leading to the best spectral match, generally using non-negative least squares. This can be extended by means of pre-calculating the solution space and using a search algorithm. If the total number of chromatic paints in the palette is nine, the number of all three-paint combinations is 84. If each paint concentration varies from 0% to 100% in 5% increments, there are 1771 entries forming the solution space. This last approach was used in this research. The concentration precision of 5% was sufficient, based on comparison of spectral RMS errors with continuous and quantized concentrations for the 20 measurement spots of *The Starry Night*.

2.3. Pigment Mapping of an Image

2.3.1. Practical Issues

It is practically difficult to perform pigment mapping pixel-by-pixel for a large image because of the limitation of computation time and memory allocation. Most programs cannot handle a large file (>2 Gigabytes) due to memory limitation. If the running time of pigment mapping per pixel using the search method is about 0.5 second, the running time for an image with 22 Mega-pixels is roughly 128 days, which is obviously unacceptable. Moreover, correlation or similarity among neighboring pixels should always be considered when mapping of an image. One approach is to accelerate the running time of pigment mapping for a single pixel. For example, the image is first segmented based on chromatic information, and for each cluster, a limited number of paints are selected to perform pigment mapping pixel-wise, which eliminates the exhaustive search for the best paint combination. The underlying assumption is that the similar colors are painted with a certain combination of paints. This approach was successfully tested with a small oil painting (less than 100 Kilo-pixels).[17] For an even larger image (22 Mega-pixels), a more practical approach should be used. Pigment mapping is only performed on a limited number of selected pixels, and pigment composition of the other pixel is assigned with the composition of one of those selected pixels that is the most similar to the pixel of interest. The main assumption of this approach is that these selected pixels should represent all the pixels in the painting. An obvious side-effect of this approach is that unwanted posterization, also known as banding, occurs in the pigment maps, which results in an abrupt change of concentrations from one region to another. The only way to alleviate this side-effect is to increase the number of the selected pixels to perform pigment mapping, which in turn increases the computation time.

2.3.2. New Practical Approach

This new practical approach takes advantage of both image classification and similarity among neighboring pixels, and also considers the balance among computation time, resolution and accuracy. It can be separated into five successive modules. Each module will be discussed sequentially.

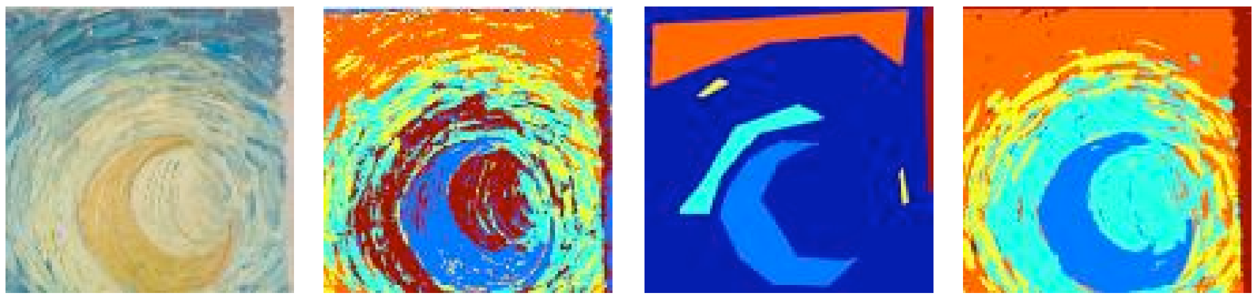
(1) Image Partition

First, the large image was divided into several small images spatially depending on the number of pixels in the large image and capacity and access time of computer memory. Modules (2) and (3) described below were repeated for each small image. For each target, two camera images and one rendered sRGB image were partitioned. Two camera images were used to calculate reflectance factor pixel-wise and similarity between pixels. The rendered sRGB image was used to facilitate selecting training regions for supervised classification.

(2) Image Classification

Second, each small image was segmented into several clusters. The classification can be done either with or without supervision. Unsupervised K-Means classification[18] iteratively updates the center of each cluster until the change is negligible, so this algorithm is generally slow. In addition, the algorithm is very sensitive to the selection of initial centers and may not converge. On the other hand, supervised classification algorithms first estimate discrimination functions among clusters based on some training pixels, and then classify each pixel based on the calculated values of these discrimination functions. These algorithms involve the observer's experience for defining training pixels; however, it is computationally efficient. The simple linear classifier[18] was used.

An example of the moon image (480x482 pixels) in *The Starry Night* was given, and the classification was done in six-channel camera space. The running times on a PowerBook G4 for supervised and unsupervised methods were 6s and 207s, respectively. The classified images for these two methods are compared in Fig. 2. The supervised method successfully separated the moon, the canvas and three kinds of brushstrokes (yellow, blue-green and dark blue), based on the training pixels provided by an observer. Conversely, for the unsupervised K-Means method, the moon and canvas were classified into the same group, and the three types of brushstrokes were not separated accurately. Supervised classification segmented the image faster based on the observer's intention, so it was superior to the unsupervised method for this specific application.



(a) Original Image (b) Unsupervised Classifier (c) Training Regions (d) Supervised Classifier

Fig. 2. Comparison of supervised and unsupervised classifiers for the moon image in *The Starry Night*

(3) Pigment Mapping

Pigment mapping was only done on a limited number of selected pixels, and paint composition for the other pixels was assigned with the composition of one of the selected pixels that was the most similar to the pixel of interest. For each small image, about 1000 pixels were selected by uniformly sampling in a color space, e.g. CIELAB. The camera signals of twelve neighboring pixels surrounding each selected pixel (no more than 2-pixel Euclidean distance) and the selected pixel were averaged to represent this selected pixel in order to reduce camera noise. After that, reflectance factors for these selected pixels were calculated from their camera signals. The paint composition for each selected pixel was determined using the search method.

Each small image was classified into several clusters with the supervised linear classifier. The camera signals were extracted for the first cluster, and the selected pixels that belonged to this cluster were also extracted. The similarity metric was the simple Euclidean distance between two pixels in six-channel camera space. The distances between each pixel and all the selected pixels in this cluster were calculated. The paint composition of the selected pixel that was the most similar to the pixel of interest was assigned to that pixel. The whole process was repeated for all the pixels in this cluster and then for the next cluster until all of the clusters were processed. The output was a series of pigment maps for each small image.

(4) Image Combination

After that, the next step was to stitch pigment maps for all small images into a large image for each material.

(5) Image Rendering

Finally, the image was rendered from these pigment maps along with the optical properties of these paints for a specific combination of illuminant and observer, the same as the image rendered from the two camera images. These two rendered images were compared on a display or on paper, and visual inspection was used to evaluate colorimetric performance of the image rendered from these pigment maps. An image-based color difference formula should be considered in future.

Other useful applications can also be done with these pigment maps. For example, if the optical properties of darkened paints before fading are known, the color appearance of the original painting can be simulated with these pigment maps and the optical properties of these unfaded paints. These pigment maps provide valuable historical knowledge of the painting and could also aid conservators for retouching the damaged areas in the painting.

3. RESULTS and DISCUSSION

3.1. Determination of van Gogh's Palette

The artist's palette was approximated using six oil pigments selected from the Gamblin Conservation colors and four other pigments, the selection based on contact spectrophotometric measurements and *a priori* analytical research[15] on one of his self-portraits, executed during the same time period. The white paint was lead white, measured from Georges Seurat's *A Sunday Afternoon on the Island of La Grande Jatte – 1884*.[19] The use of lead white paint is not common nowadays because lead is poisonous and lead paint will become discolored over a long period time. The green pigment was emerald green that had the most beautiful and the most intense green color, but it is chemically unstable and contains arsenic. Three blue pigments – cobalt blue, ultramarine blue and Prussian blue – were selected. Both cobalt blue and ultramarine blue were used by van Gogh based on the contact spectrophotometric measurements of several paintings from this time period. Prussian blue was incorporated to account for the difference between modern and van Gogh's blue paints. Four yellow pigments were selected based on spectral curve shape analysis, cadmium lemon yellow, zinc yellow, Indian yellow and earth yellow. The last pigment in the palette was burnt sienna. It was found from pigment mapping that this pigment was largely used to predict red and dark colors. It was known that this artist did not use black pigment in his paintings, so no black pigment was chosen.

3.2. Performance of Camera System

The camera system was a Sinarback 54 camera with two optimized filters, and set up perpendicular to the painting. Two fluorescent light sources with a correlated color temperature of 4460 K were placed 45° on either side of the optical path. The transformations from camera signals to reflectance factor were built with a ColorChecker DC (abbreviated as CCDC) using the Matrix R method.[5] Average color differences (CIEDE2000) for CCDC and 20 measurement spots on the painting were 1.2 and 3.6 ΔE_{00}, respectively, while the mean spectral RMS errors were 1.6% and 2.5% in that order. Both spectral and colorimetric accuracies were comparable to previous experimental results,[5] and the retrieved reflectance factor was accurate enough to find the pigment compositions of each pixel.

3.3. Performance of Pigment Mapping

Pigment mapping was performed based on single-constant K-M theory, where the optical property was the ratio between absorption and scattering coefficients for each paint calculated from one reflectance measurement. The mapping method used was the search, and the best three-paint combination plus white paint along with their optimal concentrations was found to match each pixel with the smallest spectral RMS error between measured and predicted reflectance factors.

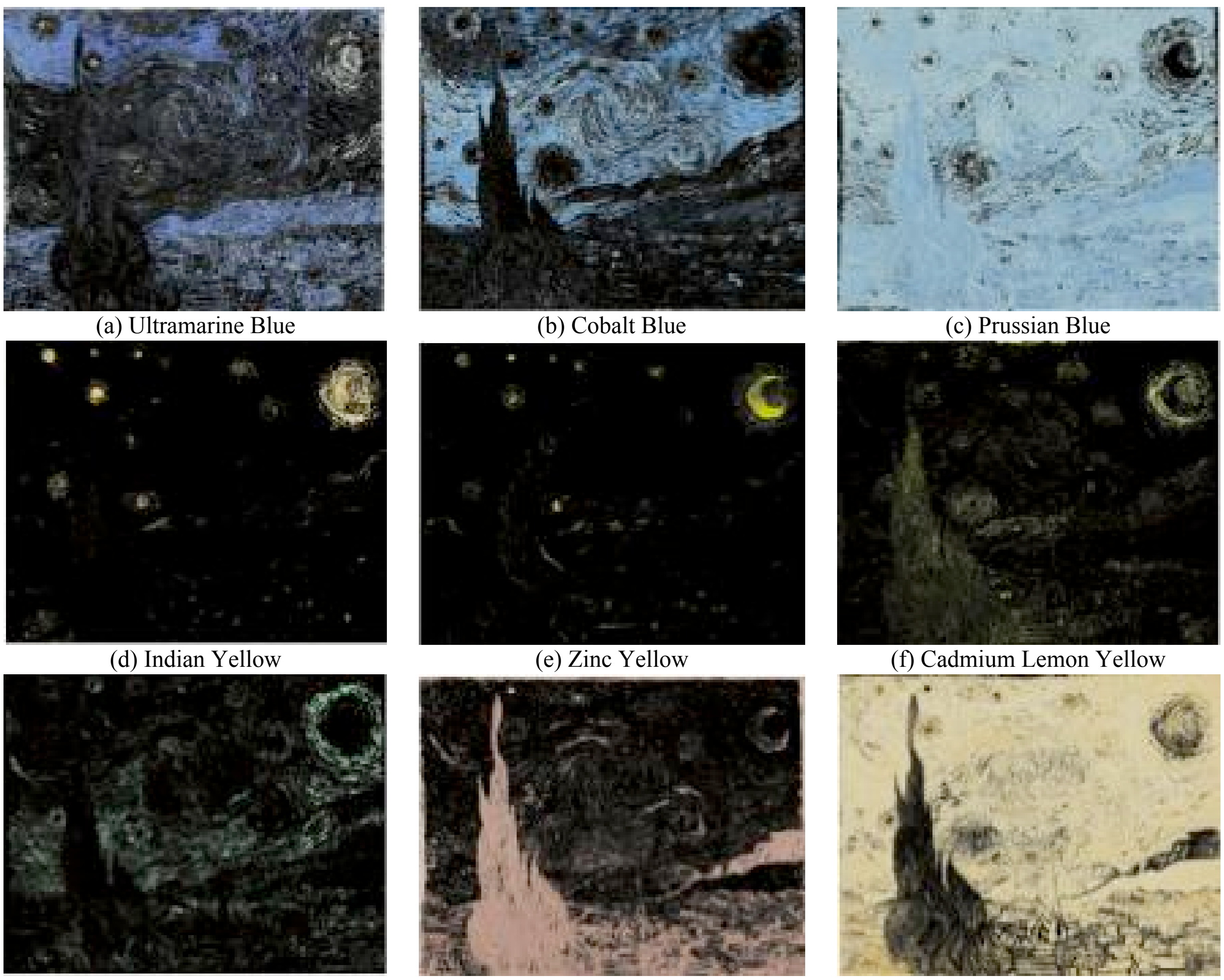
Pigment mapping was done for 20 measurement spots of the painting. It was found that predicted reflectance spectra could follow these measured ones very closely. The mean color difference for these spots was 3.2 ΔE_{00}, and mean spectral RMS error was 1.9%. Both colorimetric and spectral accuracies of pigment mapping were comparable or slightly superior to those accuracies of camera prediction. It proved that simplified single-constant model and opaque assumption were acceptable. Next, the inaccuracy of camera prediction was considered, and pigment mapping was done with predicted reflectance factors from camera signals for these spots. The prediction accuracies of pigment mapping based on contact spectrophotometric measurements and spectral-based camera were not statistically different. It further confirmed that the spectral accuracy of the camera system was sufficient for pigment mapping.

3.4. Pigment Maps

The output was a series of spatial concentration maps of pigments consisting of the painting, as shown in Fig. 3. For better visualization of these maps, the concentration values were color-coded. The concentration value of one was displayed as the color of pure paint or masstone, and zero concentration was shown as the black color. The concentration value between zero and one was coded with the tint color of the paint mixed with white paint.

The large areas of blue sky were undoubtedly painted with both ultramarine blue and cobalt blue. The region of blue sky where the stars were located contained, predominantly, ultramarine blue while the swirling sky and region surrounding the moon contained, predominantly, cobalt blue. Emerald green, used in light bluish-green brushstrokes surrounding the moon, was not used to create the dark green in the cypresses. The moon and stars were most likely created with Indian yellow and zinc yellow. Cadmium lemon yellow might be used to paint the yellow clouds surrounding the moon and the stars. The cypress tree might be painted with burnt sienna and Prussian blue. The maps of Prussian blue and earth yellow indicated that a small amount of these two paints was used almost everywhere in the painting, which was very unlikely. These two maps had a low credibility, but their existences certainly helped improve the prediction accuracy of pigment mapping. One possible reason is due to obvious spectral difference between modern and old paints, and these two paints might be used to compensate this difference. Spectral characteristics of old paints could be estimated from the contact spectrophotometric measurements of the painting and used in the pigment mapping. Another possible reason might be the inaccuracy of the single-constant K-M theory based on the assumption that the scattering is dominated by the white paint only. If both the absorption and scattering coefficients of paints in the palette are characterized, more accurate pigment mapping based on two-constant K-M theory should be used. More importantly, it implied that one or more paints used by the artist were not identified, and the discovery of the unknown paints requires further modern analysis techniques, e.g., X-ray fluorescence spectroscopy and microscopy of cross sections.

The image rendered from the pigment maps was compared with the image calculated from camera signals for the same illuminant and observer on a high-resolution LCD. Overall, the two images were similar. The reproduction from the pigment maps was slightly pale, and had unwanted banding in some regions. It was caused by the practical approach of pigment mapping; for each small image, pigment mapping was done only on a limited number of pixels, and the other pixels were mapped based on similarity with these selected pixels. The blue sky in the top-left corner of the reproduction from these pigment maps lacked the purple blue color (the color of pure ultramarine blue), although pigment mapping successfully identified this pigment in that region. In addition, it was found that this color exhibited perceptible color change with the change of illuminants and observer, which made it difficult to judge the color appearance of the rendered images on a display. Considering the practical camera system, the simplified pigment-mixing model and the practical approach for pigment mapping of a large image, pigment mapping of *The Starry Night* was satisfactory.



(a) Ultramarine Blue (b) Cobalt Blue (c) Prussian Blue

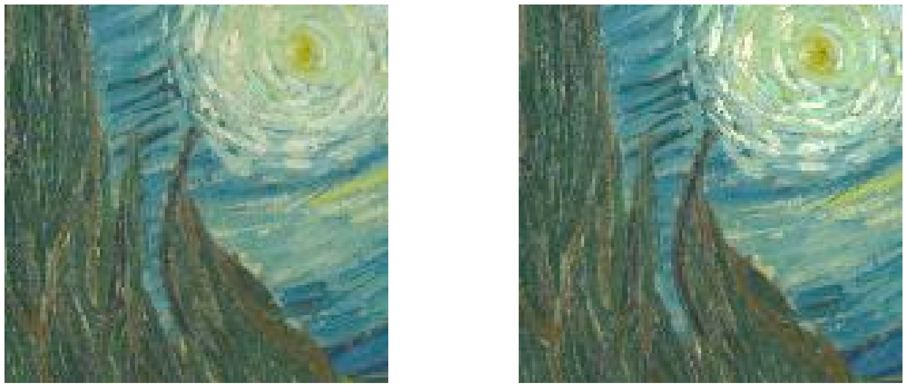
(d) Indian Yellow (e) Zinc Yellow (f) Cadmium Lemon Yellow

(g) Emerald Green (f) Burnt Sienna (i) Earth Yellow

Fig. 3. Pigment maps for the painting *The Starry Night*.

3.5. A Simulation with "Fresh" White Paint

These pigment maps made it possible to digitally rejuvenate the color appearance of the paining if the white paint had not darkened. The color appearance of *The Starry Night* was simulated when the optical property of "aged" lead white (darkened) was replaced with that of "fresh" one (a modern dispersion of lead white in linseed oil). A small part of the painting before and after rejuvenation is shown in Fig. 4. These two images had dramatic differences around the star. The lightness of these colors surrounding the star increased significantly when "fresh" lead white was used.



(a) "Aged" lead white (b) Fresh lead white

Fig. 4. Simulated images with the optical properties of both aged (a) and fresh (b) lead white

4. Conclusions

Vincent van Gogh's *The Starry Night* was extensively studied. Van Gogh's palette was approximated using six oil pigments selected from the Gamblin Conservation Colors and four additional oil colors based on contact spectrophotometric measurements and *a priori* analytical research on one of his self-portraits, executed during the same time period. A practical pigment mapping method was applied to the spectral image of this famous painting. It was found that the region of blue sky where the stars were located contained, predominantly, ultramarine blue while the swirling sky and region surrounding the moon contained, predominantly, cobalt blue. Emerald green, used in light bluish-green brushstrokes surrounding the moon, was not used to create the dark green in the cypresses. Indian yellow and zinc yellow were used to paint the moon and stars. Cadmium lemon yellow might have been used to paint the yellow clouds surround the moon and the stars. The maps of Prussian blue and earth yellow indicated that a small amount of these two paints was used almost everywhere in the painting, which was very unlikely. This means that the approximated palette can be improved. The pigment maps were used to simulate the painting's appearance before the natural ageing of lead white dispersed in linseed oil. Considering the practical camera system, the simplified pigment-mixing model and the practical approach for pigment mapping of a large image, pigment mapping of *The Starry Night* was very satisfactory. Pigment mapping based on spectral imaging was found to be a viable and practical approach for analyzing pigment composition, and providing new insight into an artist's working method, the possibility for aiding in restorative inpainting, and lighting design.

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