Improvement of Spectral Imaging by Pigment Mapping

Yonghui Zhao, Roy S. Berns, Yoshio Okumura, and Lawrence A. Taplin, Munsell Color Science Laboratory, Chester F. Carlson Center for Imaging Science, Rochester Institute of Technology, Rochester, New York, USA

Abstract

Spectral imaging has been widely developed over the last ten years for archiving cultural heritage. It can retrieve spectral reflectance of each scene pixel and provide the possibility to render images for any viewing condition. A new spectral reconstruction method, the matrix R method, can achieve high spectral and colorimetric accuracies simultaneously for a specific viewing condition. Although the matrix R method is very effective, the reconstructed reflectance spectrum is not smooth when compared with in situ spectrophotometry. The goal of this research was to smooth the spectrum and make it more accurate. One possible solution is to identify pigments and find their compositions for each pixel. After that, the reflectance spectrum can be modified based on two-constant Kubelka-Munk theory using the absorption and scattering coefficients of these pigments, weighted by their concentrations. The concentrations were optimized to best fit the spectral reflectance predicted by the matrix R method. As a preliminary experiment, it was assumed that a custom target was painted using several known pigments. The simulation results show that incorporating pigment mapping into the matrix R method can recover the smoothness of the reflectance spectrum, and further improve spectral accuracy of spectral imaging.

Introduction

Traditional colorimetric devices acquire only three samples, critically under-sampling spectral information and suffering from metamerism. Alternatively, spectral devices increase the number of samples and can reconstruct spectral information for each scene pixel. Retrieved spectral information can be used to render color images for any viewing condition. Spectral imaging has been widely developed over the last ten years for archiving culture heritage at a number of institutes worldwide. Three spectral acquisition systems have been developed and tested in our laboratory.[1]

Recently, the matrix R method was proposed and implemented for spectral imaging reconstruction.[2-3] The method followed the Wyszecki hypothesis[4-6] where a spectrum can be decomposed into a fundamental stimulus and a metameric black. The spectral reflectance and tristimulus values were both calculated from multi-channel camera signals. Then the hybrid spectral reflectance was generated by combing the fundamental stimulus and metameric black predicted from tristimulus values and spectral reflectance, respectively. This method achieved high spectral and colorimetric accuracies simultaneously for a certain viewing condition. The spectral accuracy of this method was mainly determined by the estimated spectral reflectance, which was calculated by multiplying the multi-channel camera signals with a transformation matrix. Each column of the transformation matrix can be estimated by a basis vector, and spectral reflectance can be represented as a linear combination of these basis vectors, weighted by the multi-channel camera signals. A transformation matrix for a six-channel virtual camera is shown in Figure 1. Due to the wavelike shape of the basis vectors, the predicted spectral reflectance for a white patch, for examples, is not as flat as *in situ* spectrophotometry, shown in Figure 2. The goal of this research was to smooth reflectance spectra and to further improve spectral accuracy.

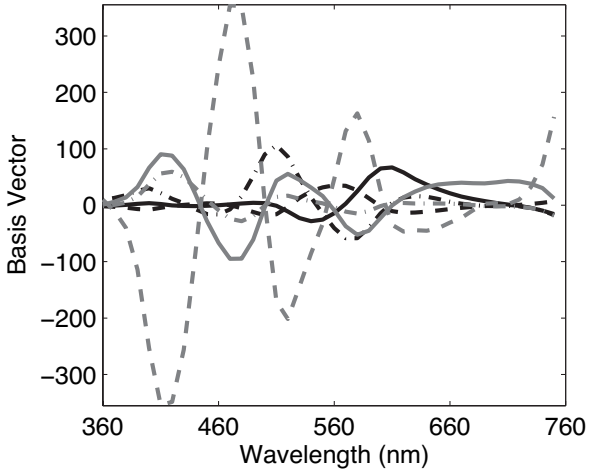

Figure 1. The transformation matrix from six-channel camera signals to spectral reflectance factor.

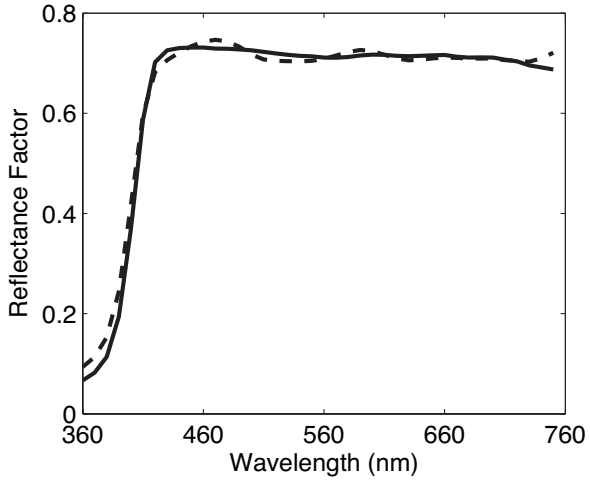

Figure 2. Measured (solid) and predicted (dashed) spectral reflectance factors for a white object.

Praefcke proposed a method to smooth basis vectors by taking the roughness of basis vectors into account in the optimization.[7] In his method, these basis vectors were actually eigenvectors of a reflectance database, and the first eigenvector explains the most variability of the database, and the second eigenvector explains the second most variability of the database, and so on. The cragged shapes of the forth and fifth eigenvectors are related to both the least variability of the database and the noise associated with the database. The transformation matrix used in the matrix R method, however, is quite different from the eigenvectors in the Praefcke's method. The column vectors of the transformation matrix are almost equally significant and cannot be smoothed using the Praefcke's method.

Another approach is to analyze the composition of each pixel, and incorporate the pigment information into the prediction of spectral reflectance. Pigment identification usually requires more information than just visible spectral reflectance.[8-10] As a pilot experiment, it was assumed that the pigments composed of a paint target were known. This research bypassed pigment identification and directly performed pigment mapping using the known pigment database. In 1931, Kubelka and Munk[11] proposed a turbid media theory that derived the nonlinear relationship between colorant concentration and spectral reflectance for a translucent colorant layer. Allen[12] applied the Kubelka-Munk theory for colorant formulation and developed a series of numerical methods. For this research, the painting was assumed to be opaque. Two-constant Kubelka-Munk theory was used to describe the nonlinear relationship between spectral reflectance and colorant concentration. The colorant concentrations were optimized to best fit the spectral reflectance predicted by the matrix R method. Next spectral reflectance was reconstructed from the colorant concentrations and the pigment database. Finally, the smoothed reflectance was used to calculate the metameric black that was combined with the fundamental stimulus. The preliminary results show that incorporating pigment mapping into the matrix R method can smooth reflectance spectra and further improve spectral accuracy.

Theory

Pigment Mapping

The general mathematical model of Kubelka-Munk theory for translucent samples is rather complicated, but two simplified models could be derived from the general model for the cases of transparent and opaque film with opaque support. Since the paint sample used in this research was largely opaque, the relevant equations are:

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda,mix} = \frac{\left(1-\mathbf{R}_{\lambda,mix}\right)^2}{2\mathbf{R}_{\lambda,mix}} \tag{1}$$

$$\mathbf{R}_{\lambda,mix} = 1 + \left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda,mix} - \sqrt{\left(\frac{\mathbf{K}}{\mathbf{S}}\right)^2_{\lambda,mix} + 2\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda,mix}} \tag{2}$$

where $\mathbf{R}_{\lambda,mix}$ is the spectral reflectance of a pigment mixture and $(\mathbf{K}/\mathbf{S})_{\lambda,mix}$ is the ratio of spectral absorption ($\mathbf{K}$) and scattering ($\mathbf{S}$) of the mixture, which can be further expressed using the amount of pigments (c), the number of pigments (n), the absorption ($\mathbf{k}$) and scattering ($\mathbf{s}$) of pigments at unit amount.

$$\left(\frac{\mathbf{K}}{\mathbf{S}}\right)_{\lambda,mix} = \frac{c_1\mathbf{k}_{\lambda,1} + c_2\mathbf{k}_{\lambda,2} + \mathbf{L} + c_n\mathbf{k}_{\lambda,n}}{c_1\mathbf{s}_{\lambda,1} + c_2\mathbf{s}_{\lambda,2} + \mathbf{L} + c_n\mathbf{s}_{\lambda,n}} \tag{3}$$

$$\sum_{i=1}^{n} c_i = 1$$

The first and most important step is to develop the colorant database, which includes the unit absorption and scattering for each pigment. The tint ladder of each pigment is a certain number of mixtures of the pigment with white paint. If there are two samples in the tint ladder, in which case n is equal to 2 in Eq. (3), the absorption and scattering of the pigment at unit amount can be solved simultaneously. Otherwise, the unit absorption and scattering of the pigment can be solved by the linear least squares method, and further optimized to minimize the average RMS error between measured and predicated reflectances for the tint ladder. Then, spectral reflectance of an unknown target is predicted by Eqs. (2) and (3) using all the pigments in the database. If the unknown target is a mixture of these pigments in the database, the predicated spectral accuracy is high; otherwise, there is no guarantee that good prediction can be achieved. For this research, it was assumed that the concentration threshold is 5% according to some prior knowledge about the unknown target. That is to say, the pigment was removed from the composition of the unknown target if the predicted concentration for this pigment was below the threshold. The pigment concentrations of the unknown target were optimized to minimize the weighted RMS error[13] between measured $\mathbf{R}_\lambda$ and predicated spectral reflectance $\mathbf{R}_\lambda$ (m accounts for the number of wavelengths). Since human visual system is more sensitive to mismatches in dark colors than light colors, the weighted RMS error is to weight spectral data with small magnitude more than the ones with larger magnitude.

$$wRMS = \sqrt{\frac{\sum_{\lambda=1}^{m}\left[\sqrt{1/\mathbf{R}_\lambda}\left(\mathbf{R}_\lambda - \hat{\mathbf{R}}_\lambda\right)\right]^2}{m}} \tag{4}$$

The reflectance measurement is affected by the interface between air and the opaque layer and this index of refraction discontinuity can be corrected by the Saunderson equation.[12] For sphere geometry with specular included, the relationship between measured reflectance $\mathbf{R}_{\lambda,m}$ and internal reflectance $\mathbf{R}_{\lambda,i}$ can be expressed in the following two equations.

$$\mathbf{R}_{\lambda,i} = \frac{\mathbf{R}_{\lambda,m} - k_1}{1 - k_1 - k_2 + k_2\mathbf{R}_{\lambda,m}} \tag{5}$$

$$\mathbf{R}_{\lambda,m} = k_1 + \frac{(1-k_1)(1-k_2)\mathbf{R}_{\lambda,i}}{1 - k_2\mathbf{R}_{\lambda,i}} \tag{6}$$

The two parameters in the Saunderson equation were predefined as $k_1 = 0.03$ and $k_2 = 0.6$ according to a previous analysis. All the spectral reflectances were corrected using Eq. (5) and then transformed to $(\mathbf{K}/\mathbf{S})_{\lambda,mix}$ by Eq. (1).

Virtual Camera Model

A virtual camera model[2] was used to test the method. Six-channel camera signals were computer-generated to simulate a traditional color-filter-array (CFA) digital camera combined with two absorption filters. The spectral sensitivity of the entire camera system for each channel $\mathbf{S}_{\lambda,i}$ can be expressed as the product of spectral transmittances of the absorption filter, $\mathbf{F}_{\lambda}$, and infrared cut-off filter, $\mathbf{I}_{\lambda}$, and the spectral sensitivity of the detector for the channel, $\mathbf{C}_{\lambda,i}$.

$$\mathbf{S}_{\lambda,i} = \mathbf{F}_{\lambda}\mathbf{I}_{\lambda}\mathbf{C}_{\lambda,i} \tag{7}$$

For an object with spectral reflectance $\mathbf{R}_{\lambda}$, a camera signal for each channel, $\mathbf{D}_i$, is calculated by Eq. (8):

$$D_i = \sum_{\lambda=1}^{m} \left(\mathbf{R}_{\lambda}\mathbf{E}_{\lambda}\mathbf{S}_{\lambda,i}\right) + \eta_i \tag{8}$$

where $\mathbf{E}_{\lambda}$ is the spectral power distribution of the illuminant and η_i is a noise term.

Matrix R Method

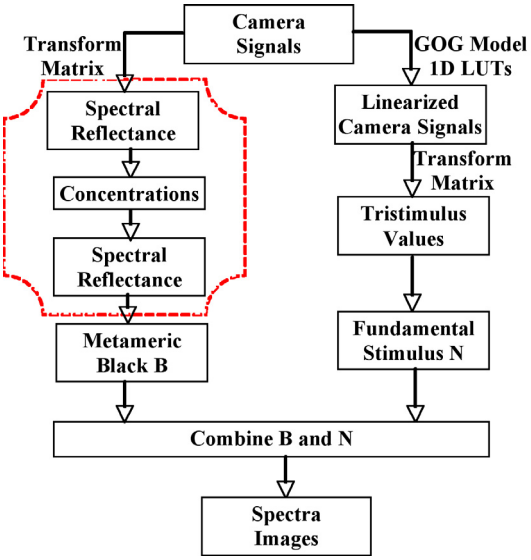

Figure 3. Flowchart of the matrix R method with pigment mapping.

The matrix R method combines the benefits of spectral and colorimetric transformations. First, as illustrated in the right branch of the flowchart, the camera signals are linearized using the gain-offset-gamma (GOG) model, commonly used to characterize CRT displays, and then converted to tristimulus values. These tristimulus values are used to calculate the fundamental stimulus. Second, along the left branch of the flowchart, spectral reflectance is estimated from the same camera signals using a transformation matrix. Pigment mapping is incorporated next, indicated by the dashed line in the flowchart. The concentrations of pigments are estimated from predicated spectral reflectance, which are then used to calculate the smoothed spectral reflectance. For this modified version of the matrix R method, the smoothed reflectance is used to calculate the metameric black. Finally, the hybrid reflectance can be calculated combining the metameric black and the fundamental stimulus.

Experimental

In this experiment, the virtual camera was a Sinarback 54H color-filter-array (CFA) digital camera combined with two absorption filters. The spectral sensitivities of the entire camera system are plotted in Figure 4, and the HMI light source was measured using a Photo Research PR704, shown in Figure 5.

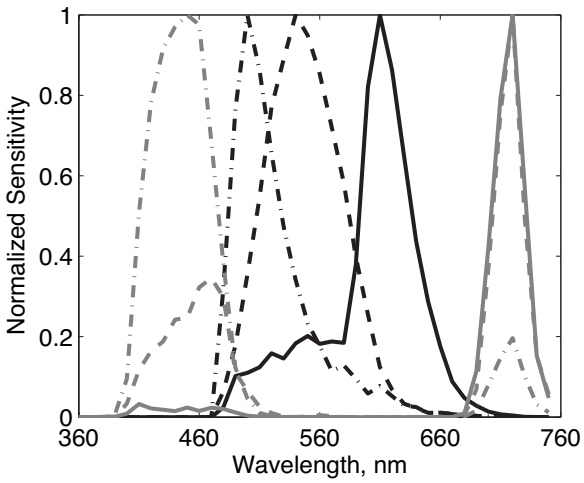

Figure 4. Spectral sensitivities of the entire camera system.

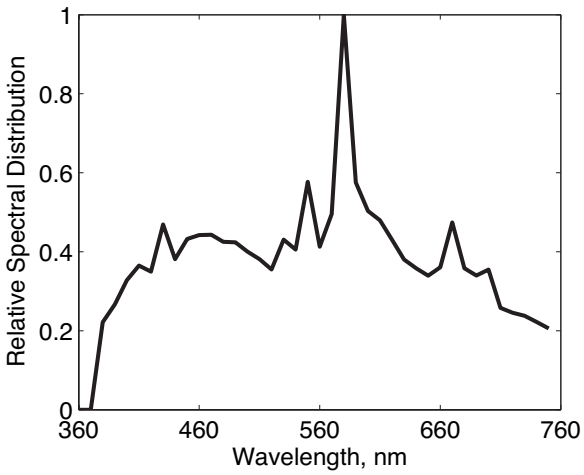

Figure 5. Spectral power distribution of the HMI light source.

The GretagMacbeth ColorChecker DC was used to calibrate the camera model, which included a transformation matrix from camera signals to spectral reflectance, six 1-dimensional (1D) look-up-tables (LUTs) to linearize the camera signals, and another transformation matrix from the linearized camera signals to tristimulus values, as shown in the flowchart above.

Another target was a custom target of Golden artist colors, abbreviated as the Golden target in the following discussion. This

target was made of titanium white and three colored pigments – hansa yellow opaque, pyrrole red and ultramarine blue. There were forty-five patches in this target. The first eighteen patches were tint ladders for the three colored pigments. The next nine samples were mixtures of two colored pigments without white paint. The last eighteen samples were mixtures of two colored pigments with white paint. All these samples were carefully prepared and measured using a GretagMacbeth ColorEye XTH sphere spectrophotometer with specular component included.

Results and Discussions

Pigment Mapping

In this section, the accuracy of pigment mapping was tested based on two-constant Kubelka-Munk theory. The Golden target was made up of the known recipes. The concentrations were predicted using nonlinear optimization to minimize the weighted RMS error between measured and predicated spectral reflectances. The error metric for pigment mapping was the squared Euclidean distance between the known and predicated recipes. Table I lists the statistical results of the error metric for the pigment mapping. The algorithm successfully identified the number of pigments in each patch and determined their concentrations. The mean concentration error was 3.1%, but the maximum error was 15.7%. It was found that the errors were high for two colorant mixtures without white paint, corresponding to patch Nos. 19-27. It might be caused by the accuracy of two-constant Kubelka-Munk theory or lack of opacity for the paint samples. The existence of white paint improved the accuracy of the concentration determination. If patch Nos. 19-27 were excluded, the mean error reduced to 1.0%, indicating a very successful pigment mapping.

Table 1: Statistical Results for Pigment Mapping (%)

Statistics	Mean	Std. Dev.	90% percentile	Min	Max
All patches	3.1	4.6	11.0	0.0	15.7
Excluding patch Nos. 19-27	1.0	1.2	1.9	0.0	5.1

The spectral reflectance can be estimated from both the known and predicted recipes using Eqs. (2) and (3). Figure 6 compares measured and estimated spectral reflectances with the spectral RMS error indicted in the legend. The estimated spectral reflectance from the predicted recipe had a smaller spectral RMS error than that from the known recipe. This was expected since the predicted recipe was optimized to minimize the RMS error between the measured and estimated spectral reflectances. Noticeable discrepancies were observed between the measured and estimated spectral reflectance from the known recipe. Such discrepancy might be caused by the accuracy of the Kubelka-Munk model. Other possible reasons might include measurement error, lack of opacity, non-uniformity of the paint sample, and numerical error.

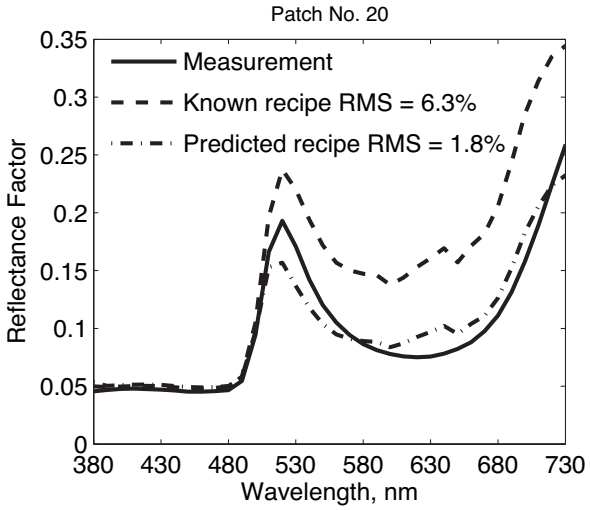

Figure 6 Measured spectral reflectance (solid) and estimated spectral reflectance using the known (dashed) and predicted (dotted) recipes.

Original Matrix R Method

In this section, both the spectral and colorimetric accuracies of the matrix R method are provided in detail. The colorimetric error metric includes color difference CIELAB and CIEDE2000 under CIE illuminant D65 and for 2 degree observer, while the spectral error metric includes spectral RMS error and two metamerism indices that consist of both a parametric correction for CIE illuminant D65 (A) and color difference CIEDE2000 under CIE illuminant A (D65).

Table 2: Colorimetric and Spectral Accuracies for Calibration Target – GretagMacbeth ColorChecker DC (CCDC) – Between Measured and Predicted Spectral Reflectances

CCDC	ΔE_{ab}	ΔE_{00}	% RMS	MI (D65>A)	MI (A>D65)
Mean	1.06	0.69	1.48	0.24	0.30
Std. Dev.	0.82	0.43	0.81	0.63	0.70
90% percentile	2.29	1.36	2.30	0.38	0.51
Min	0.07	0.07	0.08	0.01	0.01
Max	4.31	2.42	4.83	9.34	10.17

Table 3: Colorimetric and Spectral Accuracies for the Golden Target Between Measured and Predicted Spectral Reflectances Without Pigment Mapping

Golden	ΔE_{ab}	ΔE_{00}	% RMS	MI (D65>A)	MI (A>D65)
Mean	1.86	1.02	3.84	0.91	1.09
Std. Dev.	1.34	0.64	1.34	0.74	0.85
90% percentile	3.97	2.01	5.61	2.09	2.68
Min	0.17	0.14	1.49	0.08	0.07
Max	5.28	2.64	6.02	2.92	3.49

Table 2 and 3 list the statistical results of the colorimetric and spectral error metrics for the calibration target and the custom target. It can be seen that colorimetric performances for both targets were very good. It means that nonlinear optimization to minimize color difference is an effective technique to improve colorimetric performance. However, spectral accuracy is unsatisfactory. For example, the mean spectral RMS error for Golden target was 3.84%, and the maximum metamerism index for the ColorChecker DC was very high. Figure 7 compares predicted spectral reflectance for the virtual camera model with *in situ* spectrophotometer for two patches in the Golden target using the original matrix R method. The method has some degree of difficulty in matching the long wavelength reflectance "tail" of the ultramarine blue (bottom).

Improved Matrix R Method

The original matrix R method can be improved by incorporating pigment mapping. The predicted spectral reflectance by the original matrix R method from the six-channel camera signals were used to estimate the concentrations of pigments for each patch, which were used to calculate spectral reflectance using Eqs. (2) and (3). This approach, as indicated by the statistical results in Table 4, didn't change colorimetric performance, but as expected, significantly improved spectral accuracy. The mean RMS error decreased from 3.8% to 1.1%, and the maximum RMS error was reduced almost two fold. The two metameric indices also decreased appreciably.

Table 4: Colorimetric and Spectral Accuracies for the Custom Target – Golden Target – Between Measured and Predicted Spectral Reflectances with Pigment Mapping

Golden	ΔE_{ab}	ΔE_{00}	% RMS	MI (D65>A)	MI (A>D65)
Mean	1.86	1.02	1.05	0.25	0.36
Std. Dev.	1.34	0.64	0.48	0.22	0.26
90% percentile	3.97	2.01	1.66	0.47	0.64
Min	0.17	0.14	0.27	0.00	0.01
Max	5.28	2.64	2.35	0.83	1.13

Figure 7 illustrates the improvement of spectral accuracy by pigment mapping for two selected patches of the Golden target. For the white patch (top), the predicted reflectance by the improved matrix R method almost overlapped with the measurement. The improvement was even more pronounced for the ultramarine blue (bottom), where the predicted reflectance with pigment mapping followed much more closely with the measurement. It is then obvious that pigment mapping improves the spectral accuracy of the original matrix R method.

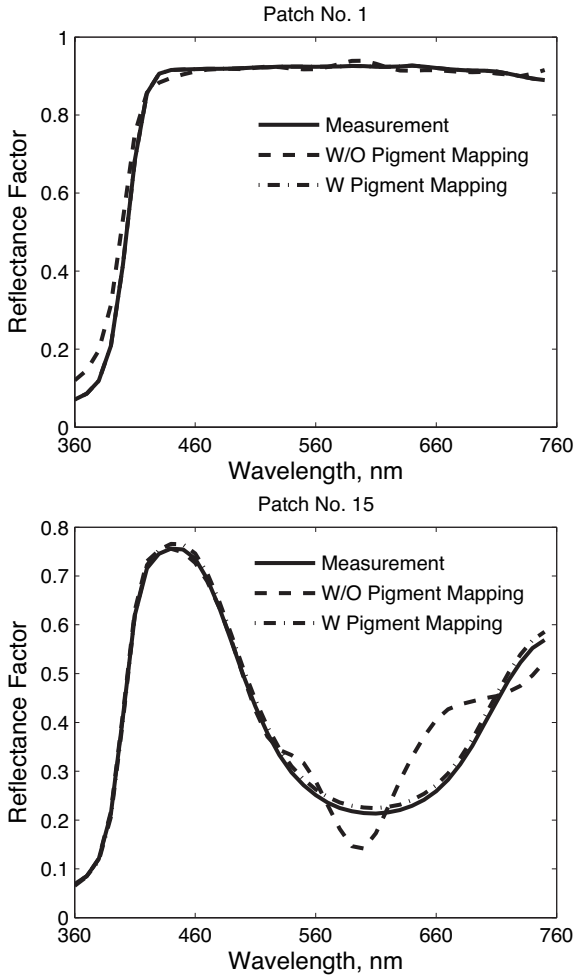

Figure 7. Spectral accuracy of the six-channel virtual camera without pigment mapping (dashed) and with pigment mapping (dash dotted) compared with in situ spectrophotometry (solid) for two selected patches of the Golden target.

Conclusions

Compared with conventional color imaging, spectral imaging takes advantage of much more embedded information in spectral reflectance. The original matrix R method combines the benefits of both spectral and colorimetric imaging, and it can provide a highly accurate match to an original target, both spectrally and colorimetrically. The spectral accuracy of the matrix R method can be further improved by pigment mapping. A virtual camera model was simulated and used along with a custom target of Golden artist colors to verify the recovery of the smoothness of spectral reflectance predicted by the original matrix R method. Incorporating pigment mapping reduces the mean spectral RMS error for the custom target from 3.8% to 1.1% and the maximal RMS by almost two fold. It also decreased the degree of metamerism appreciably. In conclusion, by incorporating pigment mapping, the improved matrix R method can achieve even higher spectral accuracy.

Acknowledgments

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Author Biography

Yonghui Zhao is a PhD candidate of imaging science in the Munsell Color Science Laboratory at Rochester Institute of Technology. She received her B. S. and M. S. degree in material engineering from Dalian University of Technology, China. Her research interests include spectral-base color reproduction, color management solution, pigment identification and pigment mapping.