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Instrumental inter-agreement study of spectral and colorimetric data of a new multi-angle spectrophotometer

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Abstract:

The visual appearance of goniochromatic materials is very attractive but it is also difficult to measure them to get a complete characterization. During last years, different instruments have appeared in the market with the purpose to obtain a good color characterization in different measurement configurations, the multi-angle spectrophotometers. These commercial devices have different optical configurations and different working mechanisms. However, the measurements provided by each instrument would be similar to have a good consistency. Therefore, after the release of a new multi-angle-spectrophotometer, the CM-M6 from Konica-Minolta, the purpose of this work is to apply an inter-agreement study of spectral and colorimetric data of three instruments (CM-M6, BYK-mac-i and MA98) in order to guarantee a good performance between instruments. Two different statistical tests were applied following ASTM recommendations. The proposed tests were the Hotelling's test and the statistical intercomparison test and a set of 91 goniochromatic samples were considered. In general, the measurement geometries close to the specular direction (aspecular angle equal to -15° and 15°) and the flop direction (aspecular angle equal to 110°) show greater deviations. In addition, the partial color differences calculated for the comparison MA98 vs. CM-M6 are larger than for the BYK-mac-i vs CM-M6 comparison. Finally, from the statistical results, it can be concluded that

most of the measurement geometries are statistically significant which means that these differences are due to systematic or bias errors but not exclusively to random errors.

Keywords: color measurement, goniochromatism, spectrophotometry, reproducibility, inter-model-agreement

INTRODUCTION

From past century, the use of goniochromatic or special-effect pigments^{1, 2} has exponentially grown in many modern industries, from the automotive sector^{3, 4}, as a pioneer, to others (coatings, cosmetics, dentistry⁵, plastics⁶, printing⁷⁻⁹, textiles¹⁰, etc.). In the last years, different color-measuring instruments, multi-angle spectrophotometers, were developed to measure and characterize special-effect pigments (metallic, interference, pearlescent) in many materials with a particular visual appearance. The visual appearance of a material with these special-effect pigments is very attractive since the color appearance changes with changes in the illumination and observation directions (goniochromatism). In addition, they provide visual texture effects (gloss¹¹, sparkle¹² or glitter or glint, coarseness¹³ or graininess, pearliness¹⁴, etc), and therefore it is required complex instrumentations to completely characterize these materials, and to propose efficient models of visual

and instrumental correlation for detection, scaling and discrimination (including tolerances^{15, 16}). Thus, in many cases, a conventional optical setup¹⁷, typically used in classical spectrophotometers or based on color-imaging systems^{18,19}, both for diffuse or directional geometries, is not completely efficient for color management in these industries (automotive, etc.)

In general, a multi-angle spectrophotometer characterizes the gonio-color appearance by measuring the spectral relative reflectance factor and the CIELAB values of the sample with different illumination and observation angles^{20, 21}. However, from a point of view of optical measurement of materials, this is an approximation well extended in color industry using goniochromatic materials because the main source of optical and spectral data is the BRDF concept²²⁻²⁴. For goniochromatic materials, from metallic to interference and diffractive effects²⁵, the main challenge for color instrumentation manufacturers is to measure correctly with the minimal number of geometries^{26, 27} to obtain the maximum spectral and colorimetric information, i.e. predicting accurately the complete BRDF, and the corresponding color palette of any goniochromatic material²¹. However, this is not trivial because it means to take into account the structural information^{28, 29} (flake orientation, measurement geometry into the flake particle, etc.) to understand and manage pro-actively its macro-optical and visual impact. Thus, although from several international optical metrology institutes there are some calibrated multi-angle-spectrophotometers^{30, 31} available, with capability to measure from several tens to thousands of measurement geometries, the current trend in color industry is to save time and measure right and efficiently^{32, 33} to obtain and manage the maximum optical and visual information for quality management.

In nowadays markets, there are different multi-angle spectrophotometers with different characteristics and specifications belonging to different companies. For instance, BYK-Gardner launched the BYK-mac instrument in 2009, nowadays updated to a new version BYK-mac-i. The BYK-mac-i multi-angle spectrophotometer provides the CIELAB values under the D65 illuminant at 6 different measurement geometries. These six illumination-detection geometries are designed by CIE as 45°x:-60°, 45°x:-30°,45°x:-20°, 45°x:0°, 45°x:30° and 45°x:65°, respectively or regarding the specular direction as 45°:as-15°, 45°:as15°, 45°:as25°, 45°:as45°, 45°:as75° and 45°:as110° where the negative/positive sign of these six angles indicate clockwise/counterclockwise rotation angles with respect to the specular reflection of the incident light. The measuring area of this instrument is a diameter of 23 mm . X-Rite company developed a

multi-angle spectrophotometer in 2008, the MA98 multi-angle spectrophotometer. This device has two illumination angles, 15° and 45°, with a total of 19 measurement configurations, both in and out-of-plane. The measurement area is around 12 mm in diameter. In the same way, and released in 2016, Konica Minolta has developed a new multi-angle spectrophotometer: the CM-M6. This instrument is characterized by a new lateral double illumination system at 45° for minimizing colorimetric errors caused by positioning error in multi-angle measurements with an area of measurement of 12 mm. A possible irregular geometry of its optics has been corrected³⁴. Therefore, the main purpose of this study is to evaluate the instrumental inter-model-agreement of the spectral and colorimetric data of the new multi-angle spectrophotometer from Konica Minolta with regard to other current commercial multi-angle spectrophotometers available in the market in order to guarantee a good performance between instruments.

METHODOLOGY

For this study the ASTM E2214-17 normative, valid for any color-measuring instrument^{35, 36}, and here for multi-angle spectrophotometers, was applied following a previous work³⁷.

In particular, the comparison was performed between an X-Rite multi-angle spectrophotometer (MA98), the last version of the BYK multi-angle spectrophotometer (BYK-mac-i) and the new multi-angle spectrophotometer from Konica-Minolta (CM-M6). These instruments share 6 common measurement geometries: 45°x:-60° (as -15°), 45°x:-30° (as 15°), 45°x:-20° (as 25°), 45°x:0° (as 45°), 45°x:30° (as 75°), 45°x:65° (as 110°). Regarding the illumination direction, CM-M6 was used with the double illumination system at 45°. However, X-Rite and BYK-mac instruments illuminate from the left side. It is important to mention that all the instruments were used with its standard configuration, the most used on the industry, thus the direction of illumination considered for CM-M6 was double illumination. In the same way, the BYK-mac configuration for the measurement area was 23 mm and not 12 mm.

The ASTM E2214³⁶ standard specifies different specific statistical studies based on the comparison of average values to analyze the inter-model-agreement. In this way, only instrument differences between pairs of instruments can be evaluated. The proposed test are the Hotelling's test and the statistical intercomparison test to determine the confidence interval of the partial color differences ΔL^* , Δa^* , Δb^* , and the total color difference ΔE^*_{ab} . A wide set of samples, composed by 91 metallic and interference samples were measured by the three instruments. This set

of samples was measured 20 times without replacement. The spectral reflectance factors were measured by considering each instrument. Then, the colorimetric data were calculated from each multi-gonio spectrophotometer for the CIE D65 illuminant and the CIE standard colorimetric observer by using Matlab® following the same methodology that in the previous work³⁷. The average values were then considered in order to conduct the reproducibility study.

By considering the previous work, the CM-M6 instrument was compared with the other multi-angle spectrophotometers. Firstly, the partial and total color differences were calculated in the CIELAB color space. For a perfect reproducibility between instruments, all color differences would be zero. Secondly, a statistical study of the reproducibility comparison between devices was conducted by calculating the average and mean square deviation of the colorimetric values. In particular, Hotelling's T^2 test describes the acceptance volume of an instrument in terms of ΔL^* , Δa^* , and Δb^* relative values. This is a multivariate metric that indicates the tolerance volume of an instrument for a given statistical significance. T^2 is calculated from a given sample's color difference data and the population covariance matrix (S) of color difference data:

$$S = \begin{bmatrix} \text{var}(\Delta L^*) & \text{cov}(\Delta L^*, \Delta a^*) & \text{cov}(\Delta L^*, \Delta b^*) \\ \text{cov}(\Delta L^*, \Delta a^*) & \text{var}(\Delta a^*) & \text{cov}(\Delta a^*, \Delta b^*) \\ \text{cov}(\Delta L^*, \Delta b^*) & \text{cov}(\Delta a^*, \Delta b^*) & \text{var}(\Delta b^*) \end{bmatrix}$$

$$T^2 = n \cdot [\Delta L^* \ \Delta a^* \ \Delta b^*]^T \cdot S^{-1} \cdot [\Delta L^* \ \Delta a^* \ \Delta b^*]$$
(1)

where the superscript T indicates matrix transpose and n is the number of measurements. Each T^2 value can be tested for significance with a given a probability by using the F-distribution:

$$F_{3,n-3} = \frac{(n-3)T^2}{3(n-1)} \quad (2)$$

The second test is based on series of pairwise comparison tests based on statistics obtained from propagation of errors and the Chi-squared statistical distribution. This test calculates the $g_{i,j}$ coefficients to compute interval estimates for the component differences, ΔL^* , Δa^* , and Δb^* . In the equation 3 is the form for the statistical test:

$$\alpha = \frac{\text{mean}(\Delta L^*)}{\text{mean}(\Delta E_{ab})}, \quad \beta = \frac{\text{mean}(\Delta a^*)}{\text{mean}(\Delta E_{ab})}, \quad \gamma = \frac{\text{mean}(\Delta b^*)}{\text{mean}(\Delta E_{ab})}$$

$$g_E = g_{11}\alpha^2 + g_{22}\beta^2 + g_{33}\gamma^2 + 2g_{12}\alpha\beta + 2g_{23}\beta\gamma + 2g_{13}\alpha\gamma$$

$$t_{\Delta E} = \sqrt{\frac{\chi_3^2}{n \cdot g_E}}, \quad n = 91 \quad (3)$$

where χ^2 is the chi-square value for 3 degrees of freedom. Regarding the critical value $t_{\Delta E}$, it can be concluded if there exists a good inter-model-agreement between instruments since from this value it can be established if the total color differences ΔE_{ab}^* are statistically significant. That is, if the average is higher than the critical value ($\Delta E_{ab}^* > t_{\Delta E}$), the difference is significant, i.e. for that directional geometry the measurement data, the found errors are systematic errors which produce consistent errors due to different factors related to the instruments (angle tolerances for each geometry, photometric scales, white standards, etc.), but are not caused by unknown and unpredictable changes in the measurement (random errors).

RESULTS

This methodology was then applied to know the instrument difference between 2 pairs of instruments:

1. CM-M6 vs. BYK-mac i
2. CM-M6 vs. MA98

It is important to mention that the analysis was conducted by considering the 91 samples. However, with the first analysis, some problems were found for some samples due to the small size of these samples. For this reason, only samples with a size bigger than the instrument apertures were considered for this paper. The new "subset" was composed by 49 samples.

To analyze the instrument differences, firstly, CIELAB color differences (Δb^* vs. Δa^* and ΔL^* vs. ΔC_{ab}^*) were plotted to know the behavior of individual samples. Figures 1 to 2 show the CIELAB color differences for different pairs of comparisons.

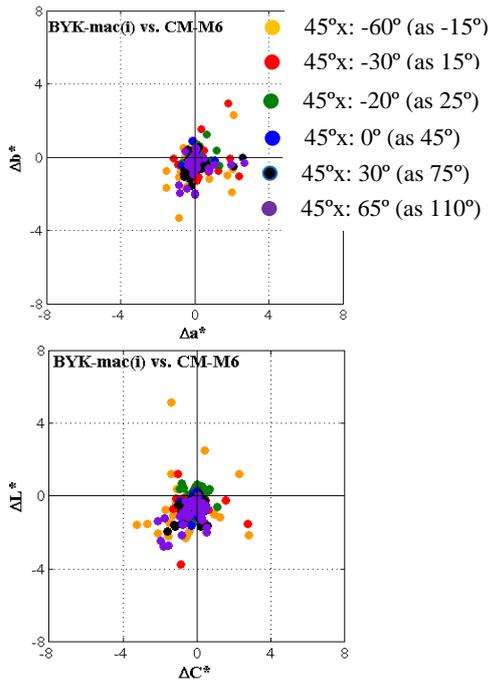


Figure 1. CIELAB color differences (Δb^* vs. Δa^* and ΔL^* vs. ΔC_{ab}^*) for the inter-comparison pair CM-M6 and BYK-mac-i.

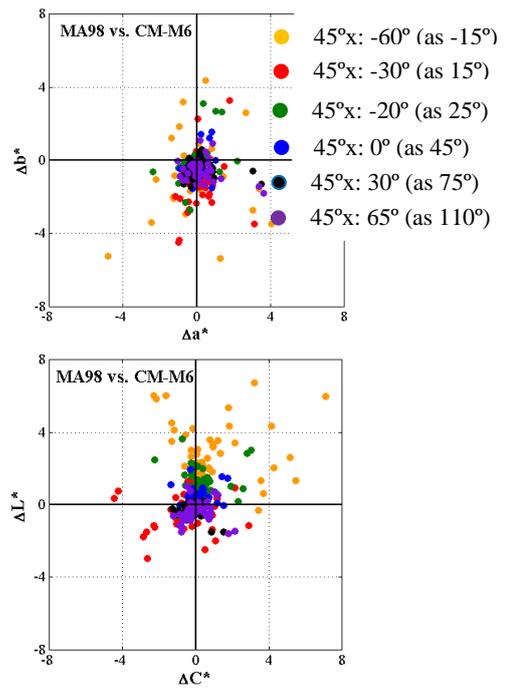


Figure 2. CIELAB color differences (Δb^* vs. Δa^* and ΔL^* vs. ΔC_{ab}^*) for the inter-comparison pair CM-M6 and MA98.

From the previous figures, in general for all the measurement geometries, the dots are broadly spread around the color difference space. However, the measurements obtained for the geometries $45^\circ x: -60^\circ$ (as -15°) and $45^\circ x: -30^\circ$ (as 15°), close to the specular angle, are more broadly spread than for the other geometries, which can be expected due to the interference and metallic nature of the samples.

To complete this analysis, the results of the colorimetric intercomparison are collected in Table 1. The average of the partial color differences, ΔL^* , Δa^* and Δb^* , and the maximum and minimum values of these partial color differences, are shown for each comparison. By considering the mean value, the partial color differences are smaller than 1 for all the color attributes except for the b^* coordinate for the MA98 vs. CM-M6 comparison at measurement geometries close to the specular direction. In general, the partial color differences calculated for the comparison MA98 vs. CM-M6 are larger than for the BYK-mac-i vs CM-M6 comparison.

Table 1. Average, maximum and minimum values of the partial color differences obtained for each measurement geometry.

		<i>MA98 vs. CM-M6</i>			<i>BYK-mac-i vs. CM-M6</i>		
		Mean	Max	Min	Mean	Max	Min
45°as-15°	ΔL^*	2.78	6.73	0.30	1.07	5.19	0.08
	Δa^*	0.89	4.79	0.05	0.54	2.11	0.01
	Δb^*	1.28	5.39	0.02	0.66	3.34	0.01
45°as 15°	ΔL^*	0.79	2.99	0.00	0.70	3.77	0.02
	Δa^*	0.63	5.45	0.01	0.38	2.40	0.00
	Δb^*	1.45	4.51	0.26	0.51	2.94	0.02
45°as 25°	ΔL^*	1.23	3.63	0.2	0.34	1.53	0.00
	Δa^*	0.48	2.35	0.01	0.27	1.35	0.00
	Δb^*	0.63	3.1	0.02	0.25	1.23	0.00
45°as 45°	ΔL^*	0.45	1.94	0.01	0.65	1.65	0.11
	Δa^*	0.24	1.02	0	0.19	1.10	0.00
	Δb^*	0.43	1.55	0.01	0.31	0.91	0.02
45°as 75°	ΔL^*	0.27	1.53	0.00	0.52	1.94	0.08
	Δa^*	0.41	3.49	0.00	0.30	2.59	0.01
	Δb^*	0.43	1.44	0.02	0.38	1.59	0.03
45°as110°	ΔL^*	0.48	1.58	0.01	0.91	2.79	0.01
	Δa^*	0.47	3.62	0.00	0.30	2.70	0.00
	Δb^*	0.61	1.82	0.01	0.57	2.04	0.03

On the other hand, to evaluate the color differences more closely, another graph was plotted. Figure 3-5 shows a bar representation of each partial color difference for three measurement geometries (45°as-15°, 45°as45°, 45°as110°) to know there is a systematic deviation for all the samples. Regarding the comparison with the BYK-mac-i instrument, it can be checked that the color differences are greater for the 45°x:-60° (-15°) measurement geometry. In general, the lightness value calculated for the CM-M6 instrument is greater than for the BYK-mac-i instrument ($\Delta L^* < 0$) in contrast to the MA98 measurement, which provides lightness values greater than the BYK-mac-i instrument ($\Delta L^* > 0$). For a* and b* coordinates is not possible to conclude any systematic error since it depends on the sample although the calculated deviation is less than for the lightness value. However, in most samples there is a deviation in the b* coordinates with the same direction ($\Delta b^* < 0$). Regarding the MA98 and CM-M6 comparison, it is more difficult to find a general tendency for any CIELAB value. Again, the deviations are greater for the measurement geometries close to the specular direction. In general, it is possible to define the same ranking for all the comparisons. That is, if the deviations or

discrepancies according the measurement geometry are considered, the same behavior is found. The measurement geometries close to the specular direction (aspecular angle equal to -15° and 15°) and the flop direction (aspecular angle equal to 110°) show greater deviations, while the differences for the measurement geometries close to the face direction (aspecular angle equal to 25° and 45°) are smaller.

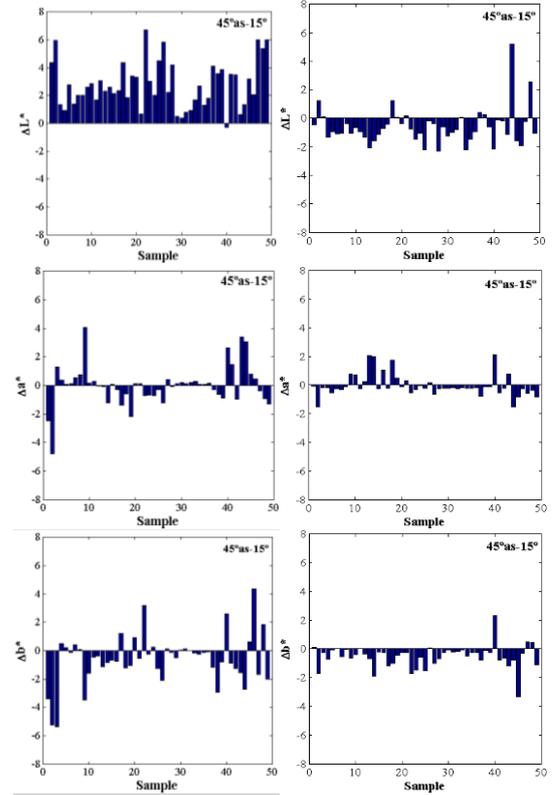
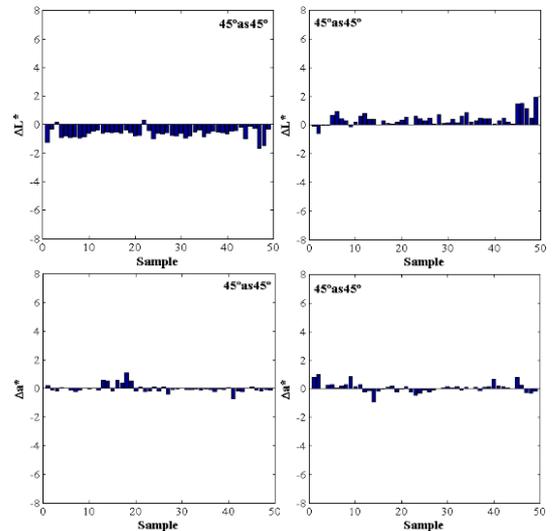


Figure 3. CIELAB color differences (ΔL^* , Δb^* , Δa^*) for the inter-comparison pair CM-M6 and MA98 (left) and CM-M6 and BYK-mac-i (right) and for the 45°:as-15° measurement geometry.



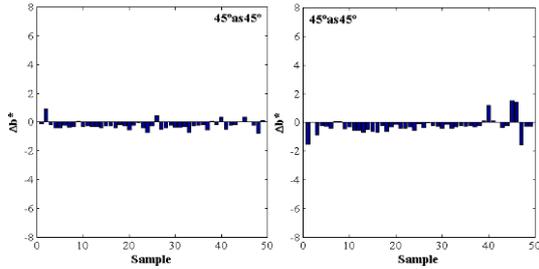


Figure 4. CIELAB color differences (ΔL^* , Δb^* , Δa^*) for the inter-comparison pair CM-M6 and BYK-mac-i (right) and CM-M6 and MA98 (left) for the 45°:as45° measurement geometry.

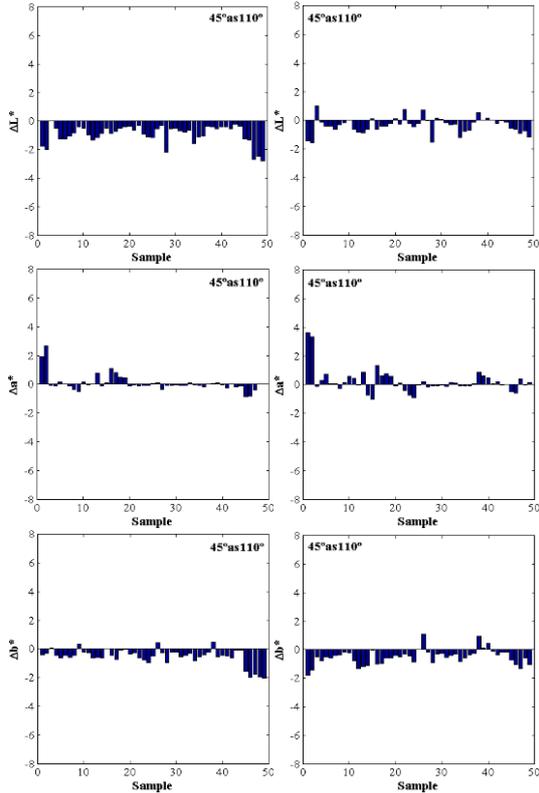


Figure 5. CIELAB color differences (ΔL^* , Δb^* , Δa^*) for the inter-comparison pair CM-M6 and BYK-mac(i) (right) and CM-M6 and MA98 (left) for the 45°:as110° measurement geometry.

In addition, the spectral data are considered to evaluate the deviations between instruments. As example, the spectral reflectance of 2 samples measured by each instrument are shown in Figure 6.

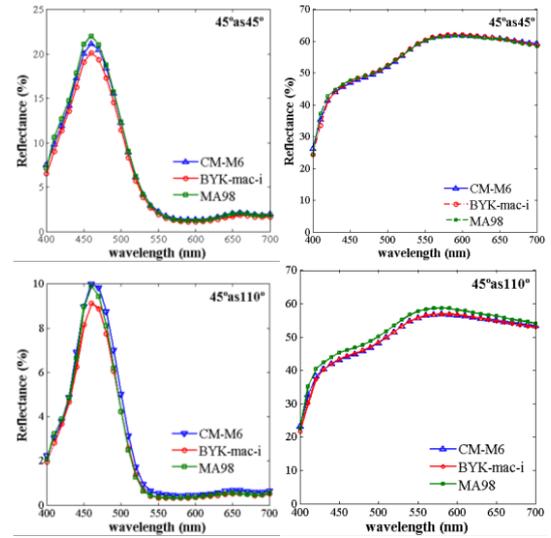
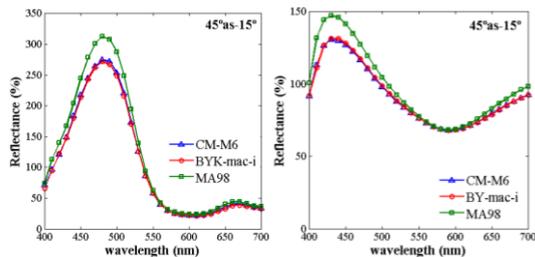


Figure 6. Spectral reflectances for the Sample #1 (*Alubrigh 3100*) (left) and the Sample #3 (*M1034S*) (right) measured by each multi-angle spectrophotometer for three different measurement geometries.

After this analysis, the statistical analysis was done to know if the deviations or discrepancies between instruments were significant. Table 2 shows the multivariate statistical results from the Hotelling' s test. The results were generated with an algorithm in Matlab software.

Table 2. Hotelling's analysis T^2 for color differences of 49 samples measured by the two studied comparisons (CM-M6 vs. MA98 and CM-M6 vs. BYK-mac-i) with a confidence interval of 95% ($\alpha = 0.05$).

Geom.	CM-M6 vs. MA98		CM-M6 vs. BYK-mac i	
	T^2	P	T^2	P
as -15°	197.35	0.000	31.566	0.000
as 15°	50.108	0.000	44.814	0.000
as 25°	157.826	0.000	3.008	0.419
as 45°	105.318	0.000	161.371	0.000
as 75°	34.526	0.000	65.339	0.000
as110°	43.767	0.000	102.574	0.000

The hypothesis tested was whether the colorimetric differences (ΔL^* , Δa^* , Δb^*) between instruments were equal to zero. The results are shown for the statistical significance of 95%, equivalent to $\alpha = 0.05$. As can be observed, for the CM-M6 and MA98 multi-angle spectrophotometer pair, the P-values for all the measurement geometries are lower than the α value. This indicates that the instruments contribute in a statistically significant way to the color difference between instruments. For the other pairwise comparison (CM-M6 vs. BYK-mac-i), some measurement geometries were found not to be

statistically significant, such as the 45°x:-20° (as 25°) measurement geometry.

The ASTM intercomparison test was conducted to determine the confidence interval of the partial color differences ΔL^* , Δa^* , Δb^* and the total color, by calculating the covariance matrix S and the critical value $t_{\Delta E}$ (in accordance with equations 3). Table 3 shows the total color differences ΔE^*_{ab} and the critical value $t_{\Delta E}$ calculated for each measurement geometry between the two pairwise comparisons. Comparing the critical value $t_{\Delta E}$ and the average of the total color differences makes it possible to determine whether the differences are statistically significant. In most of the cases, all the measurement geometries for the comparisons are statistically significant because the averages are higher than critical values ($t_{\Delta E}$), i.e. these geometries are unlikely to have occurred by chance. These results also coincide with all results previously obtained by the Hotelling's test for color differences.

Table 3: Average and critical values of the total color differences ΔE^*_{ab} obtained for each measurement geometry for the two studied comparisons (CM-M6 vs. MA98 and CM-M6 vs. BYK-mac-i).

<i>CM-M6 vs. MA98</i>						
	as -15°	as 15°	as 25°	as 45°	as 75°	as 110°
g_E	0.3328	0.2791	1.2024	3.7500	1.3520	0.8812
$t_{\Delta E}$	0.6923	0.7560	0.3642	0.2062	0.3435	0.4254
$\overline{\Delta E^*_{ab}}$	3.4787	1.9143	1.6367	0.7571	0.7219	1.0068
<i>CM-M6 vs. BYK-mac-i</i>						
	as -15°	as 15°	as 25°	as 45°	as 75°	as 110°
g_E	0.2825	0.7912	0.1876	5.1636	2.2133	1.4506
$t_{\Delta E}$	0.7513	0.4490	0.9221	0.1757	0.2684	0.3316
$\overline{\Delta E^*_{ab}}$	1.5100	1.0752	0.5721	0.7986	0.7762	1.2013

CONCLUSIONS

The main purpose of this paper was to show an inter-model-agreement study between three current types of multi-angle spectrophotometers. From the results, it can be concluded that most of the measurement geometries are statistically significant. This means that these differences are due to systematic or bias errors (angle tolerances for each geometry, photometric scales, white standards, etc.), but not exclusively to random errors. With the results, it is obvious the main differences are due to radiometric scale differences.

It is important to mention that all instruments should have optical constraints with ASTM E2194, because catalog specification of all instrument list ASMT E2194. Therefore, each manufacture has little flexibility for creating own optical geometry with complying ASTM E2194. In addition, instrument manufactures do not usually disclose "true" optical geometry of their instruments. Therefore, it is very difficult to discuss radiometric scale differences. On the other hand, since all instruments should have optical constraints with ASTM E2194, other factors can be the reason of differences: sensor sensitivity (this might be related with factory calibration), tradability, effect of stray light, not difference of optical geometry. However, the statistical tests used here are not valid for discriminating and quantifying the detected bias errors in this comparison between instruments. In particular, the measurement geometries close to the specular direction (aspecular angle equal to -15° and 15°) and the flop direction (aspecular angle equal to 110°) show greater deviations. However, the differences for the measurement geometries close to the face direction (aspecular angle equal to 25° and 45°) are smaller. This behavior is found for all the pairwise comparison evaluated (CM-M6 vs. MA98 and CM-M6 vs. BYK-mac-i). Therefore, the main purpose of this work was to prove exactly that there are differences and how large these are, as the focus in this case was making a statement regarding comparability of technology in the market, not to provide any means to reduce these differences.

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