Analysis of spectrophotometer specular performance using goniometric information

David R. Wyble
Munsell Color Science Laboratory
Rochester Institute of Technology, Rochester, NY 14623

ABSTRACT
The 1986 CIE document 15.2, Colorimetry, was necessarily broad in specifying the use of the gloss trap or specular port in integrating sphere measurements. This has led to a variety of spectrophotometer configurations that adhere to the CIE recommendation. To help users of these devices determine the performance of their instruments with respect to specular excluded measurements, a procedure has been demonstrated to quantify the effective specular port width of an integrating sphere device. The proposed procedure has been tested on four spectrophotometers, three of which use conventional specular ports of varying sizes. The specular ports of these three devices can be physically measured, however the fourth device uses an alternative method for the specular excluded measurement, and the diameter of its specular port cannot simply be measured. The procedure allows for a relative comparison of conventional devices and those using an alternative method.

Keywords: spectrophotometry, specular port, gloss

1. INTRODUCTION
The study of the effect of gloss traps on spectrophotometry is not new. For decades the color measurement community has known of potential errors that can impact these measurements without careful control and understanding of the instrument specular port configuration. (See, for example, reference 1 for an overview of spectrophotometric errors and a good list of historical references.) More recent studies have quantitatively discussed the effect specular port width can have on reflectance as well as colorimetric measurements. The present work will involve the direct comparison of spectrophotometers of various specular port configurations.

The 1986 CIE recommendation 15.2 Colorimetry contains the following guidelines on angular configuration of the diffuse illumination, 0° detection case for integrating sphere spectrophotometry:

1.4 Illuminating and viewing conditions for reflecting specimens
c) Diffuse/normal (symbol d/0):
The specimen is illuminated diffusely by an integrating sphere. The angle between the normal to the specimen and the axis of the viewing beam should not exceed 10°. The integrating sphere may be of any diameter provided the total area of the ports does not exceed 10% of the internal reflecting sphere area. The angle between the axis and any ray of the viewing beam should not exceed 5°.

The two angles mentioned specify the limit to which the location of the detection port can differ from normal (the limit is 10°) and the solid angle subtense of the detection port (the maximum half-width is 5°). We can reasonably assume that instrument manufacturers place the specular ports opposite the detection port, so the specular port may potentially be up to 10° off the normal as well. The width of the specular port is not necessarily related to the width of the detection port, so the second part of the guidelines is not relevant to the present discussion.

The only mention of the specular port is in Note 1 for section 1.4:

If a gloss trap is used, details of its size, shape, and position should be given.

Manufacturers are therefore free to select any diameter or location of specular port they choose, although they are advised to report the configuration used. Users can rightfully be somewhat confused as to the specific performance of a device, especially if they use multiple spectrophotometers with differing specular port configurations. It is reasonable to expect some metric or other means to compare the various instruments with respect to their specular excluded measurements.

* Correspondence: Email: wyble@cis.rit.edu
2. EXPERIMENTAL

2.1 Samples
The samples used in this study were plastic sheets with various roughness levels stamped into their surfaces. This results in several levels of gloss, as shown in table 1 along with the sample names that will be used throughout this work.

<table>
<thead>
<tr>
<th>Color</th>
<th>Sample Name</th>
<th>Gloss Level</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>20°</td>
</tr>
<tr>
<td>gray</td>
<td>glossy</td>
<td>49.2</td>
</tr>
<tr>
<td></td>
<td>smooth matte</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>rough matte</td>
<td>0.5</td>
</tr>
<tr>
<td>tan</td>
<td>glossy</td>
<td>56.2</td>
</tr>
<tr>
<td></td>
<td>smooth matte</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 1. Sample names and various gloss levels.

2.2 Goniophotometric measurements
To characterize the specular performance of the integrating sphere devices, we must first accurately measure the set of samples with respect to their goniophotometric attributes. Each sample was measured from $-8^\circ$ to $+75^\circ$, with $1^\circ$ increments around the specular angle and $5^\circ$ increments at off-specular angles. A schematic of the goniophotometer is shown in figure 1. The device is equipped with a diffuse light source (an integrating sphere) and a collimation lens. The sample and detector are rotationally independent; physical constraints allow for a $-8^\circ$ to $+75^\circ$ detection angles given the fixed $10^\circ$ illumination angle. The detector is a Photoelectronic PR704 spectroradiometer. The units recorded are average radiance.

The goniophotometric measurements are shown in figure 2a and 2b. Figure 2a shows matte samples and 2b shows glossy samples. Both plot measured radiance, but note that the scales vary greatly. To create the full $180^\circ$ of data, three steps were used. First, data were averaged if multiple data points were available on either side of the specular angle. Next, symmetry is assumed and data were reflected across the specular angle. Last, data were smoothly extrapolated to $90^\circ$.

Figure 1. Schematic of goniophotometer. The sample and detector are rotationally independent, allowing for independent selection of detection and illumination angles. Physical constraints limit detection angles to $-8^\circ$ through $+75^\circ$. 

![Figure 1. Schematic of goniophotometer.](image-url)
Figure 2. Goniophotometric data for all samples. (a) shows matte samples and (b) glossy samples. Note that axes in (b) have very different scales than (a).

2.3 Spectrophotometric measurements

The five samples were measured in specular included (SPIN) and specular excluded (SPEX) modes on four laboratory grade bench top spectrophotometers. These are listed in table 2 along with angular diameter of their respective specular ports. All of these instruments have spheres 150 mm in diameter. Sphere coating and internal baffling configuration vary somewhat, however all adhere to CIE 15.2 recommendations.

<table>
<thead>
<tr>
<th>Device</th>
<th>Abbreviation</th>
<th>Specular Port Width (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Datacolor Spectraflash 600</td>
<td>SF600</td>
<td>4.7</td>
</tr>
<tr>
<td>Macbeth Coloreye 7000</td>
<td>CE7000</td>
<td>3.0</td>
</tr>
<tr>
<td>BYK-Gardner The Color Sphere</td>
<td>TCS</td>
<td>3.6</td>
</tr>
<tr>
<td>Minolta 3600-d</td>
<td>3600-d</td>
<td>***</td>
</tr>
</tbody>
</table>

Table 2. Spectrophotometers used in this experiment and the angular width of their specular ports. Note that the Minolta 3600-d uses an alternative configuration, and there is no physical specular port to measure.

The Minolta 3600-d uses an alternative method for measuring specular excluded reflectance. In place of the specular port, a second lamp is used, which flashes after the main lamp has flashed. This configuration places the main detector at the specular angle when the secondary lamp is flashed. Using these two flashes, SPIN and SPEX modes are measured without replacing the sample or recalibrating the device. One could measure the diameter of the viewing port and use that as the specular port diameter. However, in terms of characterizing the performance of the specular excluded mode, we are still left with very different conditions that will not necessarily compare directly with the traditional instruments.

Reflectance measurements for specular included and excluded modes are shown in figure 3. Only a few representative samples are shown. As expected, in all cases SPIN measurements of glossy samples have almost uniformly higher reflectance factors than corresponding SPEX measurements. SPIN data from matte samples will generally be much closer to the corresponding SPEX values. Table 3 shows the average difference between SPIN and SPEX reflectance factor for each sample and instrument. These will be the target values in the search described below in Theory and Calculations. The devices all behave similarly, but the differences will allow us to infer the relative impact of their specular port configuration. Equation (1) was used for this calculation, where $n$ is the number of the samples in each reflectance factor, here $n=31$:

$$\frac{1}{n} \sum_{i=1}^{700} R_{SPIN,i} - R_{SPEX,i}$$

$$SPIN - SPEX = \frac{1}{n} \sum_{i=1}^{400} R_{SPIN,i} - R_{SPEX,i}$$ (1)
### Table 3. Average difference in percent reflectance factor for SPIN and SPEX samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>SF600</th>
<th>CE7000</th>
<th>TCS</th>
<th>3600-d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gray glossy</td>
<td>3.01</td>
<td>3.04</td>
<td>3.10</td>
<td>3.12</td>
</tr>
<tr>
<td>Gray smooth matte</td>
<td>0.56</td>
<td>0.18</td>
<td>0.11</td>
<td>0.26</td>
</tr>
<tr>
<td>Gray rough matte</td>
<td>0.43</td>
<td>0.16</td>
<td>0.10</td>
<td>0.14</td>
</tr>
<tr>
<td>Tan glossy</td>
<td>3.33</td>
<td>3.18</td>
<td>3.22</td>
<td>3.23</td>
</tr>
<tr>
<td>Tan smooth matte</td>
<td>0.20</td>
<td>0.12</td>
<td>0.18</td>
<td>0.29</td>
</tr>
</tbody>
</table>

Figure 3. Reflectance factor data for a few samples. Note that two tan curves are nearly coincident.

### 3. THEORY AND CALCULATIONS

The goal of the experiment was to determine the *effective specular port width* for each spectrophotometer. This was done by searching for the width that can account for the difference between the specular included and specular excluded measurements. Since the integrating sphere devices hemispherically illuminate the sample, the first step is to rotate the goniometric data in figure 2 about the specular angle of zero. This will create the volume of reflected light, which we can assume is what the devices measure in specular included mode. The next step is to find the radius, in degrees, of a central cylinder of that volume that accounts for the average difference between SPIN and SPEX measurements for each sample. The equations used for these calculations are as follows:

\[
\text{SPEX} = \frac{\text{sample}_{\text{total}}}{\text{prd}_{\text{total}}}, \quad (2)
\]

\[
\text{SPIN} = \frac{\text{sample}_{\text{total}}}{\text{prd}_{\text{total}}}, \quad (3)
\]

\[
[1] R = 1 - \frac{\text{SPEX}}{\text{SPIN}}. \quad (4)
\]

The equations make use of the sample volume and also the volume of a perfect reflecting diffuser (PRD). The measured radiance of the PRD is taken to be an arbitrary value and constant at all angles of detection. Note that the sample volumes are normalized to their average spectral reflectance. This was to account for the fact that the diffuse (off-specular) radiance will vary for samples without nonselective spectral reflectance. The PRD volume was normalized to unity.
The numerator of equation 2 represents the total volume of sample radiance after removing the cylinder at radius $r$. The denominator is a similar quantity for the PRD. The calculated $SPEX$ in equation 2 is therefore the relative sample volume outside the given radius when compared to the similar volume of the PRD. This is intended to simulate the results of the spectrophotometers in SPEX mode. Likewise, equation 2 models SPIN mode of the devices. Equation 3 calculates the predicted average difference in reflectance factor. Mathematically, one simply plugs in various radii into equation 2, and compares the result of equation 4 to the values in table 3. The best fitting radius will be the effective specular port width, or the radius that best accounts for the difference between SPIN and SPEX measurements.

Note that the calculated widths are not necessarily expected to equal the measured widths. Rather a reasonable relationship should exist between the two. Equations 2-4 do not precisely duplicate the workings of the spectrophotometers; in equation 4, as the radius approaches zero, SPEX/SPIN ratio approaches 1 and the average $|R|$ approaches zero. As the specular port gets smaller; the SPEX measurement approaches the SPIN measurement and the difference between the reflectance factor measurements approaches zero.

4. RESULTS AND DISCUSSION

The results of the calculations are in table 4, and are shown graphically in figure 5. The matte samples show a reasonable trend with respect to the measured port width. As discussed above, is not expected that the calculated effective port widths precisely equal the measured values. A consistent relationship is all that was expected. For the matte samples this goal has been achieved.

The glossy samples do not show a similar trend. This is likely due to the fact that nearly all of the glossy reflectance is within specular ports of all instruments, and this procedure was not sensitive enough to differentiate among the devices. It was suggested by conference attendees that including a set of semi-glossy samples might help with this differentiation.

Note that the data for the Minolta are not shown in figure 5. Without the knowledge of an abscissa, here the measured port width, it is not possible to plot these data. It was hoped that a model could be derived that would enable the placement of the Minolta data and hence the derivation of an effective specular port width for that instrument. This goal is not feasible with the existing data.

<table>
<thead>
<tr>
<th>sample</th>
<th>SF600</th>
<th>CE7000</th>
<th>TCS</th>
<th>3600-d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gray Glossy</td>
<td>1.9</td>
<td>1.9</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Gray Smooth Matte</td>
<td>7.6</td>
<td>4.2</td>
<td>3.2</td>
<td>5.1</td>
</tr>
<tr>
<td>Gray Rough Matte</td>
<td>8.3</td>
<td>5.0</td>
<td>3.9</td>
<td>4.7</td>
</tr>
<tr>
<td>Tan Glossy</td>
<td>3.7</td>
<td>3.2</td>
<td>3.3</td>
<td>3.3</td>
</tr>
<tr>
<td>Tan Smooth Matte</td>
<td>6.2</td>
<td>4.8</td>
<td>5.8</td>
<td>7.5</td>
</tr>
<tr>
<td>Actual</td>
<td>4.7</td>
<td>3.0</td>
<td>3.6</td>
<td>***</td>
</tr>
</tbody>
</table>

Table 4. Effective specular port width, in degrees, for each sample and instrument. The “Actual” row is identical to the measured ports widths shown in table 2.

5. FUTURE WORK AND CONCLUSIONS

There are several extensions of the work that should be addressed in the future. First, a model should account for possible differences in reflectance factor between the specular port white cap and the integrating sphere wall. Some instruments are also known to have spatially-nonuniform specular port white caps as well. As mentioned above, a more comprehensive sample set, including semi-glossy samples and other materials is required. These samples should be spectrally non-selective whenever possible. Ideally, the collimation beam of the goniophotometer should be set up to duplicate the behavior of the individual spectrophotometers, but it may prove impractical to both determine the device configurations and implement these on a goniophotometer.

A procedure has been shown to derive the effective specular port width of an integrating sphere spectrophotometer that can aid in the differentiation of specular excluded reflectance factor measurements across instruments of different specular port configurations. Four commercial grade bench-top spectrophotometers were evaluated, three with conventional specular ports of differing sizes and one with an alternative design. The procedure successfully showed a relationship between instruments’
specular port size and demonstrates that typical bench-top spectrophotometers, which adhere to the international recommendations specified by CIE 15.2, can be compared with respect to their specular port configurations.

Figure 4. Results from table 4 showing calculated effective specular port size vs. measured specular port size. See text for further details.

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REFERENCES