Why Do Measured Values Taken with Different Color Instruments Usually Differ? An Anthology of Color Measurement Errors

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Abstract

A paper presented by the NPIRI Color Measurement Task Force at the 1993 annual TAGA meeting reports that colorimetric measurements made with spectrophotometers manufactured by the same company and with the same geometry can differ by 0.7 to 1.7 CLab ΔE and that values from instruments made by different manufacturers with the same geometry can differ by 1.5 to 3.0 ΔE . The author of this poster has published extensively on the physical mechanisms that can cause such measurement differences. This poster paper illustrates the nature of these mechanisms along with other error producing phenomena such as wavelength error, thermal and light exposure color effects, fluorescence, and transient color effects produced by flash sources.

Introduction

Density, color, and/or spectral reflectance measurement values of a given sample made with different instruments usually differ. In some cases, these differences can be explained by differences in instrument measurement geometry (e.g. differences in measured values given by an instrument with d/0 geometry and one with 0/45 geometry would not be unusual). However, color differences in the range of 0.7 to 1.7 ΔE have been observed in measurements made by instruments with the same geometry produced by the same manufacturer¹. Many of the common causes of these differences (e.g. wavelength errors) have been reported in the literature²⁻⁸. However, when small areas are measured (e. g. 5 mm square graphic arts print control strips) some additional error mechanisms affect the measured values⁹⁻¹³. In this poster presentation the nature of the mechanisms that cause data differences are described along with possible methods for their correction.

Descriptions of Measurement Difference Mechanisms

In some cases, the presence of one error mechanism can prevent the correction of differences caused by another error mechanisms. These mechanisms will be examined first. In the following section, each error source will be described and, when available, a method for determining and correcting for its presence in the measurement data taken with a given instrument will be discussed.

Lateral Diffusion Error

When light strikes the surface of most non-metallic samples most of it penetrates the air/sample interface and is scattered within the sample structure below the surface. The light that re-emerges from below the surface is, by definition, the diffusely reflected light. (Light that does not re-emerge from the surface is either absorbed or transmitted through the sample.) In this reflection process, some of the light is scattered laterally before it re-emerges as reflected light. The increase in the size of this "reflection region", relative to the illuminated area, is a function of the translucency of the sample. If the instrument measuring the reflected light does not view all of the area that the light re-emerges from, the measured reflectance value is in error. This has been referred to in the literature as edge loss³ or translucent blurring⁵ error. For the purposes of graphic arts measurement, the author has found that the term "lateral diffusion error" better describes this problem since the measured samples (e.g. paper) are not normally thought of as translucent.

This error, which is the result of a failure to measure all of the reflected light, can often be eliminated by making the area viewed by the measurement system much larger than the illuminated area or, applying Helmholtz optical reciprocity theorem, making the illuminated area much larger than the viewed area¹³. The size of the area viewed relative to the illuminated area is somewhat dependent on the depth to which the light penetrates into the sample. About 25 years ago William Voglesong determined that the size of the instrument illumination area should be 2 mm on each side larger than the viewing aperture when density measurement are being made on photographic papers. This information was subsequently incorporated into the ANSI and ISO density measurement standards¹⁴. Application of this standard cannot practically be implemented in instruments designed to measure 5 mm square print control strips¹⁰.

The method that the author has used to determine the magnitude of lateral diffusion error involves making measurements of the same sample set with several different illumination apertures and a single viewing aperture. Unfortunately, this method cannot be used with most of the small area measuring instruments on the market since they do not have provision for readily changing illumination aperture sizes. Calibrated translucent reflectance standards offer a way of determining the magnitude of the errors caused by samples of various translucencies, however, they do not solve the problem of determining the translucency of a given sample. The author is investigating this and will present results to date the 1995 TAGA meeting.

Photometric Errors

The reflectance value reported may be in error because the measuring system hardware and/or software used to determine the measured reflectance values induces errors. This can be caused by:

• Zero Error - Most laboratory instruments use a separate zero reflectance calibration. Most of the portable instruments use an internal zeroing scheme. If the means for determining the zero reflectance value is not accurate, either because of an inaccurate zero standard or an internal electronic zero error, measurements of samples with low reflectance values will be offset.

• White Calibration Error - All instruments use some sort of white standard plaque for calibration of the 100% reflectance value. Failure to keep this standard clean or degradation caused by long exposure to intense light can result in the 100% calibration of the instrument being in error. In at least one of the portable instruments, the white enameled panel as a standard contains rutile TiO₂ which only has about 20% reflectance at 400 nm. This low value, when combined with an uncertain zero value, can cause added uncertainty in the 100% value at short wavelengths.

The use of an opal glass or similar standard reference material (SRM) for standardizing a small measuring area instrument can also produce a measurement error if the lateral diffusion error is not taken into account (i. e. if the calibration values of such a SRM are determined using a large aperture laboratory instrument, it will not necessarily be the value that should be used in to calibrate a small aperture instrument). Our work with lateral diffusion indicates that the error value is roughly proportional to the square of the reflectance. Thus, a 70% SRM would exhibit half the translucency error of a 100% SRM and a 50% SRM would have roughly one quarter the error. The use of a gray standard may on occasion give less overall measurement error than the use of a white opal glass SRM.

• **Photometric Non-linearity** - The detector used to measure light intensity may not always provide an output that has a constant linear relationship to the intensity of the light falling on it. In such cases, the photometric measuring system may not give twice the output for a sample that has twice the reflectance value.

Historically, a double aperture method has been used to check for non-linearity in transmission measuring instruments. In this method, a solid sheet with two apertures is placed in the transmission cell space of the instrument. Transmission measurements are then made with one aperture blocked, then the other aperture blocked, and finally with both apertures open. Measurement system non-linearity is present if the sum of the two single aperture transmission values are not equal to the transmission value obtained with both apertures uncovered.

The structure of most modern reflectance measuring instruments, particularly portable devices with small area measurement capabilities, makes it impossible to use the double aperture method to check for photometric non-linearity. A series of very light to very dark calibrated reflectance standards can be used to determine photometric linearity. Once again, if any of these standards are translucent, they may give an inaccurate determination of photometric linearity for small area measuring instruments.

Spectral Error

The spectral analyzers (e. g. monochromators) in two instruments may not be measuring the same spectral band. This can be caused by:

• Wavelength Error - The instrument may actually be measuring spectral bands centered at wavelengths that deviate from those being reported by the instrument system. The bandpass of a single monochramator usually has a triangular shape. The effective peak of this bandpass can be shifted by a nanometer or two by combined differences in the light source spectral power distribution and the detector spectral sensitivity across the band being measured.

Some manufacturers calibrate their spectral analyzers using a laser. While this is a good tool for the manufacturing process, it does not totally satisfy the need for periodic spectral calibration in the user's environment. The spectral power distribution of a laser is not the same as the commonly used instrument light sources (i. e. usually either incandescent or xenon flash); therefore, the procedure does not detect band center shifts caused by the light source spectral power distribution. A more practical wavelength calibration for the instrument user is a set of calibrated colored ceramic tiles or plastic plaques.

• **Bandwidth Difference** - The spectral band pass of two instruments may differ. The band pass of various instruments typically range from 1 to 20 nm. However, most report data for 10 nm intervals. The algorithms used in obtaining this 10 nm reported data from the actual measured data are typically different for each instrument, but have recently been standardized by the ASTM.

Stray Light

Ideally, the spectral dispersing elements used in the instrument should pass only light in the wavelength band being analyzed. However, some light from other spectral regions can be present in the dispersed output. The output from the source and the sensitivity of the detector can vary widely over the visible range. When measurements are made in spectral regions where the source output and detector sensitivity are low, light from high source output and high detector sensitivity regions can magnify the effects of stray light errors by a factor of 100 or more. Cary 14 spectrophotomers, which the author was fortunate to use in much his earlier work, had a double monochromator system which reduced the stray light levels in the visible to between 1 part in 10^{-5} and 10^{-6} (i. e. between 0.0001 and 0.001 % of full scale). Even with this excellent performance, the possible error in some spectral regions could be as much as 0.1 %. To the best of the author's knowledge, none of the modern spectrocolorimeters use a double monochromator. Fortunately, those instruments that do use monochromators or grating-diode array systems utilize holographic gratings which exhibit stray light levels well below those of the older ruled gratings. Even so, induced stray light errors of 0.1 % or more of full scale in some spectral regions can be expected.

A few of the portable instruments use arrays of narrow bandpass interference filters as the spectral selective elements. Stray light in this case is out of band light. Tailoring the individual filters to each spectral band can result in an overall reduction of stray light error (i. e. filters used in the regions where a monochromator system would suffer most from stray light can provide tighter specifications).

Goniophotometric Induced Effects

Much of the science of photometry, particularly reflectometry, is based on the assumption a lambertian surface (i. e. the brightness of the surface is independent of the viewing angle or, put another way, the intensity of the light from a given area of the surface varies as the cosine of the viewing angle). The use of 45/0 - 0/45instruments (hereafter referred to as 0/45, -45/0 systems are fully equivalent to 0/45 systems) instead of the generally more expensive and cumbersome sphere instruments is based on the assumption that most samples are lambertian reflectors. When the angular (i. e. goniometric) distribution of the intensity of the reflected light deviates from this cosine (lambertian) function, measurements made by 0/45 and sphere instruments do exhibit large differences.

The calibration of 0/45 instruments is normally done using a diffuse reflecting SRM. The light received by the analyzer at 45° viewing is about 0.7 (i. e. the cosine of 45°) of that reflected in the surface normal direction (this ignores the 4% external reflectance that the incident beam encounters as it enters the surface). Standards with glossy surfaces are often used to, among other things, improve the durability of the standard. When reflected light with a cosine distribution below a glossy surface emerges through the surface, much of it (e.g. about 60 % for a surface that has a refractive index of 1.5) is reflected back into the SRM by the material/air interface. The amount of light transmitted through the surface varies with angle from about 96 % in the surface normal direction to 0 % at angles equal to or greater than the critical angle (e. g. about 42° for a 1.5 refractive index). At first glance, this variation in transmission with angle would seem likely to distort the angular distribution of the light as it emerged through the surface. However, a modeling of the internal reflection and transmission of the light coming through a 1.5 index

surface that the author has performed indicates that the distribution above the surface will be very nearly diffuse if the internal light angular distribution is diffuse.

Things break down when the distribution is not lambertian. For instance, if a non-scattering, absorbing layer is placed on top of a lambertian surface, the intensity of the light reflected at 45° will no longer be 0.7 of that reflected at the surface normal. In a case where the layer absorbs about 90 % of the incident light (i. e. ~ 10 % reflectance), the 45° value will be about 0.5 above a matte surfaced sample and 0.6 above a glossy surfaced sample.

Instrument Geometry Related Errors

ASTM E1164 (15) gives the standard practice for obtaining spectrophotometric data for object-color evaluation. Included in this standard are the illumination and viewing geometries for 45° reflectance: 45°/Normal (45/ 0), Normal/45° (0/45); hemispherical specular excluded reflectance: Diffuse/Normal (d/0) and Normal/Diffuse (0/d); and hemispherical specular included reflectance: Total/Normal (t/0) measurement of reflectance factor. Since most of the ASTM specifications are relatively broad (e. g. the 45° beam axis angle has a $\pm 2^{\circ}$ specification and viewing must be within 10° of surface normal in the case of d/0), it is possible for two instrument designs which meet ASTM guidelines to have considerably different optical configurations. While instrument wavelength errors may be easily detected, variations in geometry, including failure to meet the ASTM geometric specifications, cannot be so readily determined. Considering the small structures and low power light sources used in portable instruments, one may speculate that these geometry specifications are not met by some instruments. Also, the ASTM standard does not specify minimum values for light scattered by the instrument structure into the viewing optics or the illuminating and viewing aperture sizes.

Sample/Instrument Interactions

Most spectral reflectometers/photometers and densitometers are designed to have maximum accuracy when used to measure some nearly ideal sample such as a high gloss SRM. Most samples, including typical graphic arts products, exhibit considerable deviation from these ideal samples. Samples can effectively interact with the instrument to give measurement errors. Some of the physical factors of the samples that can cause these less than perfect results are:

• Fluorescence - Many manufacturers of white materials add fluorescent whitening agents (FWA) to enhance the product's apparent whiteness. These agents are generally dyes which, when excited by violet and near-UV light, fluoresce in the blue spectral region. The effect of FWA on the apparent measured reflectance values is very much dependent on the spectral distribution of the instrument illumination source. Xenon sources, which are used in some instruments, usually have much higher levels of UV relative to those of incandescent sources. Such variations in source UV can cause large variations in the apparent measured blue reflectance of samples containing FWA. While most of the fluorescence problems are related to the use of FWA, some pigments and dyes can be excited by blue light and fluoresce in the yellow, red, and even near infrared.

Determining the characteristics of fluorescent materials in samples (e. g. the emission spectra for each excitation wavelength) requires special instrumentation. Simon, Funk, and Laidlaw in an in-press paper¹⁸ discuss methods of making measurements of samples containing fluorescent dyes. The author will present a paper¹⁹ at the IS&T/SPIE electronic imaging conference, February, 1995, on the use of FWA containing white standards for determining instrument sensitivity to samples containing fluorescent whitening agents.

An anomalous triple transition type of fluorescence is occasionally observed with instruments which use flash xenon illumination sources. In normal fluorescence, a photon of the exciting source (e. g. UV) causes an electron in an atom of the material to jump to a high energy excited state. When this electron subsequently decays to its ground (i. e. stable) state, a photon with a longer wavelength than that of the exciting photon is emitted. If the intensity of the exciting radiation is very high, some of the electrons will be stimulated by two excitation photons before they can decay. This forces them into a higher energy state than that experienced in normal fluorescence. A photon with a wavelength shorter than that of normal, double transition, fluorescence is emitted when this doubly excited electron returns to the ground state.

• Light-Exposure Color (Photochromic) Effects-Some colorants change color as a function of light history. The lightening or darkening of paints and inks after long exposure to bright light is a familiar phenomenon. What is usually not realized is that when some materials are exposed to normal room light after dark storage, they will show a gradual, though reversible, color change. Most portable instruments only expose the sample to a high level illuminating source light during the measurement period. A few instruments use a shutter so that the sample is in the dark prior to measurement. This procedure gives each sample measured to a constant pattern of light history and tends to minimize error due to inconsistent light history. Storing the samples in the dark or under constant room light and using standard sample handling procedures with a deliberate pacing and timing can help to minimize lightexposure induced differences in color measurements when the instrument does not have other features to reduce photochromic effects.

Some pigments emit free, conduction electrons when irradiated with short wavelength light. This can cause the pigment composition to temporarily change. If this transient compound has different reflectance characteristics from that of the normal pigment, a change in pigment color will result. Under normal viewing light levels, the effect on the observed pigment color is very small. However, when the sample is exposed to high intensity light pulse from the illumination used in some instruments which employ flash xenon sources, a noticeable photochromic effect can be observed. One method of detecting these changes involves comparing reflectance measurements made with the flash source UV component excluded with measurements made with the UV included in the source. Using this method, the author observed a 0.3 ΔE darkening when the UV was included in the measurement of a TiO₂ (rutile) paint. A pressed pellet of a cadmium sulfide pigment showed a 0.6 ΔE darkening. While these two cases involved transient darkening of the sample, there is no reason why a transient bleaching could not occur in some compounds; a phenomenon which might be mistaken for a fluorescence effect if additional measurements were not made with a spectrofluorometer.

• Thermal Color Effects - The color of some samples and SRMs will change as the material temperature changes. The cutoff edge of high chroma red and yellow pigmented materials will often move to longer wavelengths as the temperature increases. The high levels of incandescent light used in some instruments can induce thermal color shifts when the sample is left in the measuring stage for long periods. Some laboratory instruments use thermostatically controlled heated sample holders to insure that every sample is measured at the same temperature. The use of standard sample handling procedures with a deliberate pacing and timing can help to minimize thermal induced differences in color measurements made with instruments that do not have features which minimize thermal effects.

• Surface Gloss Variations - Instruments employing the 0/d hemispherical specular excluded reflectance measurement method usually exclude the surface specular reflection by using an illuminating beam that is a few degrees (e. g. 8°) off the sample surface normal. This causes the light that is specularly reflected by the sample surface to project onto the sphere wall adjacent to port that admits the illuminating beam. If a light trap is placed at this projection point (usually done by cutting an additional port in the sphere and placing the light trap external to the sphere), then the specular component is excluded from the measured hemispherically integrated reflectance value. For this to work properly, the sample must be flat and fairly glossy in order to allow all of the specular reflected light to be captured by the light trap. If the sample surface is rippled or low gloss, then some of the specular reflected light will fall on the sphere wall and be included in the measured, specular excluded, value. Since the ASTM reflection standards do not tightly specify the geometry, instrument to instrument variations of the amount of specular light excluded can be common with some classes of samples (e. g. ink on paper).

A 45/0 instrument readily excludes the surface specular reflectance component by projecting it to a location 45° away from the viewing optics (as contrasted to 8° more or less in the 0/d instruments). In principle, these instruments should be much less affected by variations in sample gloss and flatness. However, if the areas inside the measurement head that are illuminated by specularly reflected light re-reflect that light onto the sample and/or into the viewing optics, then variations in the measured values can readily result form variations in sample gloss. This re-reflection of light is a particular problem in portable instruments which are designed to measure small areas. Generally the distances between the optical components are quite small and numerical apertures of the collection optics are relatively large.

• Sample Position - Generally, the sample to be measured is laid over the instrument measurement port or, in the case of most portables, the instrument aperture is pressed down onto the sample sheet. From the point of view of normal photometric measurement practice, a sample printed on paper should be backed with a stack of similar, unprinted paper. Measuring the sample against a relatively soft stack of paper can result in a variation in sample position which is dependent on the pressure applied to the instrument and sample stack. The author has shown in a paper published in 1993¹¹ that a one millimeter movement of the sample away from the port of one particular instrument can cause a 4 to 8 per cent change in measured value of a white sample (i. e. a 0.1 to 0.2% per 0.001" gradient). Workers in the field of photographic densitometry have found that measurements made with the sample on a rigid standard black backing provide more repeatable values. The author has also found that the use of a black backing reduces lateral diffusion error.

• **Polarization** - A paper that Franc Grum and the author published in 1973⁴ discusses the effects of sample and instrument polarization on visual and measured color. Many of the optical components used in spectrocolorimeters, particularly diffraction gratings, can partially polarize light. Samples also generally polarize the light as it emerges from their surface. The polarization of sample reflected light can interact with polarizing instrument optical components and cause measured value differences of several per cent.

The polarization of a grating monochromator is very wavelength dependent. Systems which employ bandpass filters instead of grating based spectral analyzers generally will be less sensitive to polarization. Fiber optic light pipes, which are quite commonly used in many instruments today, will generally depolarize light. Also, the use of optical components which do symmetric, coaxial illumination and light collection (e. g. an integrating sphere) will greatly reduce any effects of polarization.

Fuzzy Viewing

As pointed out in the section on lateral diffusion error, the area illuminated on the sample should be larger or smaller than the area viewed by the detector. The geometry of the illuminated and viewed areas, along with the translucency of the sample, determine the magnitude of the lateral diffusion error. With 45/0 geometry instruments, the illumination area is usually larger than the viewed area and is often defined by a solid aperture plate placed against the sample. This gives a very sharp well defined area. Generally, the smaller area is defined by the optical design. Ideally, in "perfect" optical systems, this smaller area should have a sharply defined edge. However, even with the use of the most perfect lens, the edge of the viewed area will be a little fuzzy. This ill-defined area is caused by at least two phenomena: • Optical Spread Function - The sharpness of focus of the very best lens is diffraction limited. Even an ideally perfect lens would focus a point source of light as a ringed (i. e. bulls-eye) blurry circle. The author has observed that spectrocolorimeter instrument manufacturers generally do not use high quality lenses that are corrected for spherical and chromatic aberration. The use of simple, usually high numerical aperture, lenses in instruments makes the smaller aperture (e. g. 45/0 viewing area) edge much more ill-defined.

• Scattered Light - Light can be scattered into the viewing (detection) system from the illuminating source and/or areas of the sample which are not in the desired measurement area. This is a particularly serious problem in many of the small measurement area portable instruments where the distance between optical components and the sample are very small. The author reported a procedure for determining the effect of scattered light in a 1993 paper¹¹. In this work, an instrument with a nominal 3 mm diameter circular viewing area was set to a 100% value using a white polyester sheet and to zero using glossy black glass. Next, a series of white polyester sheets with different sized holes backed by the black glass standard were measured. Each sheet was positioned to give a minimum reading. A sheet with a 6 mm hole (i. e. a 6 mm diameter black glass area surrounded by a white border) gave an 8% reading. When the lenses in the optical system were replaced with broadband anti-reflection coated lenses and other modifications were made to reduce scattered light (e. g. black paint), the reading decreased to 1%. While 1% is better than 8%, this illustrates that the system was seeing a great deal of light from outside its intended viewing area.

Computational Errors

All of the spectrocolorimeters and most of the reflectance spectrophotometers provide software routines and/or hardware for computing color coordinates and color densities from the reflected light values. ASTM E308¹⁶ specifies standard methods for computing the various CIE color coordinates from reflection data. ANSI/ASC PH2.18¹⁷ specifies standard methods for computing color densities. The computational routines supplied with the instruments may not comply with these standards. A preferred practice when evaluating various instruments is to record only the spectral reflectance data from the instrument and then use software routines based on the cited standards to compute the color and density values. This gives a computationally consistent set of values for instrument evaluation.

Conclusions

Each color instrument has its own unique set of error mechanisms and error values. If the set of error mechanisms of two instruments are the same and the values nearly coincide, we should expect the measurement values for a given sample to nearly agree. This should most likely be the case for two instruments with the same geometry made by the same manufacturer. However, even with this desirable circumstance, differences in measured values will usually exist (as is pointed out in the NPIRI paper, reference 1). Inter-instrument agreement (e. g. $0.5 \Delta E$ or better) of measured values for a set of samples is more often the exception than the rule. Tightening the specifications for standard measurement geometries would help to reduce the difference (provided that the standards where followed). However, additional specifications (e. g. scattered light) are needed if better inter-instrument measurement agreement is to be realized.

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