Best Practice Guide for Color Measurements[1]

Created during the research project „xD-Reflect: Multidimensional Reflectometry for Industry"

1. Introduction

Surface color measurements are of great importance in the production of a very wide range of manufactured goods. Industry often needs to be able to measure color within the limits of the human eye, which is about 0.5 ΔE_{ab}. A reduction in uncertainties of color measurements, ideally below 0.5 ΔE_{ab}, is needed to improve competitiveness in the trading of colored goods.
This guide tries to highlight different aspects of surface color measurements in order to obtain better measurement results. It is supposed that surface color measurements are done by using a spectrophotometer. Items that should be contained in a good spectrophotometer's calibration set, measurement error and uncertainty sources are considered. The treatment given is intended to be practical, avoiding equations as much as possible, without looking in detail to the origin of the problems, but giving solutions to them.

2. General Considerations

- Make sure the spectral bandwidth is known
- Be aware that fluorescence, if present, may influence your readings unless illumination and detection are monochromatic, in which case the effect is essentially avoided. Fluorescence is present in many objects, even in some white standards.
- Be aware that variations in temperature of the sample (thermochromism) or the instrument (e.g. amplifiers and diodes) generally influence the readings.
- The light source has to match illuminant of choice (eg. A, D_{65}, or C) as closely as possible to correctly determine color coordinates.
- Instruments have to be maintained as indicated in their manual. It is necessary to pay special attention to the handling and maintenance of the instrument's calibration standards, especially to keep them free from contamination.
- Perform the start-up routine as indicated by the instrument's manufacturer. Let the instrument warm up by a time period you have estimated to obtain stable displays/results.

3. Measurement Errors

Spectrophotometric errors are discussed in this section on a qualitative basis. All of them are known to affect the measurement result, although in different degrees for different instruments. It is the user's responsibility to check the instrument or to trust manufacturer's specification in this sense.

3.1.1. Absolute Value of the Scale

Commercial color measuring instruments usually comprise a white standard and a black standard, respectively, a light trap. These items used to calibrate instruments have an inherent uncertainty derived from their own calibration with respect to any national laboratory reflectance scale. Besides, if the items are not properly maintained (e.g. stained white standard) becomes stained, and recalibrated, the calibration factor will not be correct leading to erroneous measurements.

[1] Reproduced in parts from „Good Practice Guide to Surface Colour Measurements" by Taylor J. et al. (EUR 19552 EN (2000), ISBN: 92-828-9574-2).

3.1.2. Non-linearity of photodetector

The response of a spectrophotometer's detector to light is not always linear throughout its entire range. Towards the highest end, saturation of the detector or electronics may occur. Towards the lowest end, the noise floor will limit the minimum measurable quantity. But even in the middle range some effects may occur that modify the linear behavior normally expected. To check for this, a set of grey tiles with different reflectance values, or a set of neutral filters with different transmission values, or any other available system can be used. At least two decades should be tested. A formula, based on a polynomial, can be usually fitted for linearity correction across the range tested.

3.1.3. Angular alignment and Apertures

Some samples display a strong dependence of the color on the direction of the illumination (or the observation). This is the case if e.g. interference or diffraction pigments are embedded into the surface. In this case the results may be significantly influenced by angular deviations from the nominal measurement geometry and the size of the apertures that define the solid angles of illumination and detection may be relevant, if the spectrum changes along these solid angles.

3.1.4. Polarization

A spectrophotometers detection system may contain polarization sensitive components, such as mirrors or refraction gratings. In this case, the measurement is affected by polarization changes induced by the sample. Many samples (partially) polarize unpolarized illumination, respectively, they (partially) depolarize polarized illumination.

3.1.5. Zero Reflectance Level

Stray light and detector noise will produce a signal even if the samples reflectance was zero. Hence, the dark level signal must be subtracted from every reading. It usually happens that the dark reading changes with wavelength, which has to be accounted for.

3.1.6. Wavelength Error

Wavelength errors will lead to color errors, so the instrument's wavelength scale should be checked for. Several wavelength standards are available: spectral lamps, reflection tiles or transmission filters. The user must use the most appropriate for the instrument type.

If possible, reflectance values should be corrected according to the expression

$$R(\lambda) = R_m(\lambda) + \frac{\mathrm{d}R_m(\lambda)}{\mathrm{d}\lambda}\Delta\lambda$$

where R is the correct reflectance value, R_m is the measured reflectance value and $\Delta\lambda$ is the wavelength scale shift, the difference between the actual and the displayed wavelength. This shift can be assessed by placing a light source with a known spectral profile before the detection system. Obviously, this error cannot be checked for or corrected in those instruments, in which reflectance values are not provided to the user.

3.1.7. Spectral resolution

The spectral bandwidth used in recording the reflectance spectrum has an effect on the acquired spectral values, as it broadens and flattens spectral variations. The origin of the spectral bandwith can for instance be the width of a monochromators entry slit or the wavelength scanning speed. For many instruments this parameter cannot be set by the user, although it should be known. This source of error affects color coordinates more noticeable in chromatic samples than in achromatic ones, where the spectral dispersion is flat.

3.1.8. Sample Inhomogeneity and Anisotropy

Samples are not 100% uniform and isotropic across their surface, therefore the measurement result is an averaged value within the area covered by the luminous spot. To reduce this effect, it is advisable to average readings at different spots and to test whether rotating the samples around its surface normal produces different readings.

4. Calculation of Color Data

Calculation of color Coordinates from tristimulus values has to be done by following the recommendations of international bodies like ClE (Commission International de l'Eclairage). Tabular data for CIE Standards Observers and Illuminants are given for a 1 nm bandwidth, therefore, from a rigorous point of view they only could be used with reflectance spectra obtained using that bandwidth and that sampling interval. However, from a practical point of view, they can be used, as they are, for spectra obtained with bandwidths up to 5 nm, using a summation step of the same length. If bandwidths larger than 5 nm are used by the instrument measuring the reflectance, weighting factors shall be used for the CIE Standard Observer and Illuminant. For instance, those recommended by ASTM (American Standards for Textiles and Manufactures),.
Usually this calculation is carried out within the instrument, so it is the user's responsibility to find out whether it is correctly done or not. The amount of the error depends on the sample, but it may be as large as several ΔE_{ab} CIELAB units if a large spectral bandwidth is used.

5. Uncertainties

A measurement result will not be complete if it is not accompanied by a statement regarding its uncertainty. An adequate evaluation of the uncertainty of color coordinates is important, for example to compare results of different measurements, to establish industrial tolerances or to decide on significant differences. Currently, there is not a universally accepted method for calculating color coordinates uncertainties. However, it is assumed that at least the following uncertainty sources should be considered in the estimation of the final uncertainty. Values assigned to every one of them and the method used to compute the combined final uncertainty in color coordinates should be specified.

Sources of Uncertainty include

- White standard uncertainty.
- Photometric linearity uncertainty.
- Dark level uncertainty
- Wavelength uncertainty
- Bandwidth
- Repeatability uncertainty
- Angular uncertainty

The determination of color coordinate uncertainties can be carried out by following the current guidelines for uncertainty evaluation in metrology (Guide to the expression of Uncertainty in Measurement, GUM). The evaluation is based on a mathematical model describing the relationship of the different uncertainty sources or input quantities to the sought quantity, e.g., the color coordinates. To this end, for each input quantity an estimate and an associated uncertainty statement are specified. The combined standard uncertainty of the quantity of interest is then evaluated using the law of propagation on uncertainties (LPU). In this way, uncertainties for the tristimulus values X, Y and Z can be obtained. Since the set of tristimulus values are usually derived from the same spectral measurement the tristimulus values are often strongly correlated. In order to take this correlation into account, a covariance matrix associated to the tristimulus values can be determined by applying the methods described in GUM Supplement 2 (Evaluation of measurement data – Supplement 2 to the "Guide to the expression of uncertainty in measurement" – Extension to any number of output quantities). Subsequently the tristimulus values can be transformed to a specific color space such as (x, y, Y), (L*, a*, b*) or (L*, u*, v*) by following the corresponding transformation rules. The related uncertainty (or covariance matrix) can again be obtained by applying the LPU. When the transformation rule is non-linear (e.g. L*, a*, b*), the validity of the results can be unclear due to the linearization underlying the LPU. In this case, the obtained uncertainties can be assessed by additionally applying a Monte Carlo uncertainty analysis (Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method).