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0:45 Surface Color

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ABSTRACT

This document, SP250-71 (2007), NIST Measurements Services: 0:45 Surface Color, describes the instrumentation, standards, and techniques used to measure the surface color of reflective, non-fluorescent materials at a 0:45 geometry, that is an irradiance angle of 0° and measuring angle of 45°. The organization of this document is as follows. Section 1 describes the motivation for establishing a 0:45 Reflectometer and associated calibration services that are available. Section 2 presents the theory relevant to the measurements described in this document. Section 3 describes the 0:45 reference standard. The NIST 0:45 Reflectometer including illuminator, sample wheel, and receiver and the associated characterization and validation of the instrument are described in Section 4. Section 5 presents the sources of uncertainty and the associated analysis. A sample calibration report and reference containing details of the uncertainty method are presented as appendices.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. Introduction

The National Institute of Standards and Technology (NIST) have a long history in color and appearance, with many important contributions to our present understanding of color measurements. Interest in colorimetry at NIST dates back to the 1930's [1,2]. NIST continues to take an active role in the measurement of color with the development of the Reference 0:45 Reflectometer, henceforth referred to as the 0:45 reflectometer. The primary purpose of the 0:45 reflectometer is to disseminate color standards to the color and appearance community through a set of calibrated color tiles, British Ceramic Research (BCRA) series II*. These tiles are used to transfer the NIST 0:45 color scale to other instruments. Because color often plays a major role in the acceptability of a product, this calibration service is designed to meet a demand for improved measurements and standards to enhance the color matching of products.

The surface color of an object depends upon several factors – the spectral power distribution of the illuminant, the spectral sensitivity of the observer, the geometrical conditions of illumination and observation, and the optical properties of the object. Only the last factor depends upon the object, and is quantified by the spectral reflectance factor for opaque reflecting materials under the given geometrical conditions. Once the spectral reflectance factor is known, the tristimulus values are calculated for a given illuminant and observer, and from these values other quantities are derived, such as chromaticity coordinates and color space values.

The 0:45 reflectometer was designed to provide calibrated reflectance color standards with a target of $\Delta E^*_{ab} < 0.5$ as the primary design specification. The instrument specifications were determined by a series of simulation of errors caused by the measuring instrument on the calibrated spectral reflectance of color standard and calculated color values. Particular attention was given to the inherent properties of the instrument such as stray light, band pass error, random noise, and wavelength uncertainty. The calibrations are performed at a geometry of 0° for the irradiation angle and at a measuring angle of 45°. The calibration process is carried out by measuring the reflected flux for each sample and the reference standard for wavelength from 380 nm to 780 nm in 5 nm increments. The measurements are performed for two orthogonal polarizations and averaged. Up to 20 samples can be measured automatically during a given scan. The spectral reflectance factor for each sample is determined by the ratio of the reflected radiant flux of the sample to the reflected radiant flux of a reference standard. Once the spectral reflectance factors have been determined, the color values along with their associated uncertainties can be determined for the samples.

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* Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

The 0:45 reflectometer consists of a source section, a sample section and a detection section. The source section consists of a dual lamp housing, a double grating monochromator, and optics that direct the incident beam towards the sample. The sample section consists of a rotating sample holder which holds and positions the sample and standards in the incident beam. The detection section consists of silicon photodiodes that measure the reflected flux and monitor the incident radiation. Comparisons and check standards ensure that instrument is operating within its uncertainties on a measurement to measurement basis while periodic realizations of the scales are used to maintain the traceability of the instrument.

This document is intended to provide customers and potential customers of the 0:45 surface color measurements with a detailed overview of the capabilities and procedures used in performing the measurements. The NIST Calibration Services Program offers Service ID Number 38091S, Special Test of 0:45 Surface Color, as listed in the Surface Color and Appearance section of the Optical Radiation Measurements Chapter of the NIST Calibration Services Users Guide [3]. The measurement service quality system is based on the International Organization for Standardization (ISO), 17025 standard [4].

2. Theory

This section details the basic definitions and the relevant measurement equations to determine 0:45 reflectance factors and color values for a given measurement. The approach used in this section is based upon the concepts presented in Refs. 5-7.

2.1 Measurement Equations

According to the CIE international Lighting Vocabulary, reflectance factor is defined as the ratio of the radiant flux reflected (from a sample) in the directions delimited by a given cone angle to that reflected in the same directions by the perfect reflecting diffuser identically irradiated (same spectral composition, polarization, and geometrical distribution [8, 9]. If the cone angle is infinitely small, reflectance factor is equal to radiance factor. If the cone angle is a whole hemisphere, the reflectance factor is equal to reflectance. In this document, an infinitely small cone angle is always assumed for reflectance factor and the cone angle is not described hereinafter. The measurement of the spectral reflectance factor of a sample by the 0:45 reflectometer is performed by comparing signals from the sample and reference standard, under the same measurement conditions, at each wavelength and two orthogonal polarization of the incident radiant flux. This process is described by the measurement equation

$$R_{\mathrm{x}}(\lambda_i,\sigma)=\frac{s_{\mathrm{x}}(\lambda_i,\sigma)}{s_{\mathrm{s}}(\lambda_i,\sigma)}\cdot R_{\mathrm{s}}(\lambda_i,\sigma) \quad (2.1)$$

where λ_i and σ are the wavelength and polarization, respectively, of the incident radiation from the instrument illuminator, s_{x} and s_{s} are the measured signals from the sample and reference standard, respectively, and R_{x} and R_{s} are the reflectance factors for the sample and reference standard, respectively. The 0:45 signals from the sample and the reference standard are normalized by the signals from a monitor photodiode to account for drift in the radiant flux from the illuminator. Measurements are performed at polarizations of 0° and 90° relative to the illumination plane, so the reflectance factor of the sample for unpolarized incident radiant flux is given by

$$R_{\mathrm{x}}(\lambda_i) = \frac{1}{2}\left[R_{\mathrm{x}}(\lambda_i, 0°) + R_{\mathrm{x}}(\lambda_i, 90°)\right]. \tag{2.2}$$

A scan means measuring the 0:45 and monitoring signals for all samples and reference standards for the wavelength range of 380 nm to 780 nm at 5 nm increments and s and p polarization σ resulting in the reflectance factor for the samples. Multiple scans are used to compute the final spectral reflectance factor of the samples.

Let i index the scan, j index the reference standard, and k index the signal reading. The signals from the sample are $s_{\mathrm{x}}(\lambda, \sigma, i, k)$, the signals from the reference standard are $s_{\mathrm{s}}(\lambda, \sigma, i, j, k)$, the signals from the monitor photodiode while measuring the sample are $s_{\mathrm{m,x}}(\lambda, \sigma, i, k)$, and the signals from the monitor photodiode while measuring the reference standard are $s_{\mathrm{m,s}}(\lambda, \sigma, i, j, k)$. The average signal from the sample is

$$s_{\mathrm{x}}(\lambda, \sigma, i) = \frac{1}{l}\sum_{k=1}^{l} s_{\mathrm{x}}(\lambda, \sigma, i, k) \ , \tag{2.3}$$

where l is the number of repetitions. The equation is applied similarly for the other signals s_{s}, $s_{\mathrm{m,x}}$, and $s_{\mathrm{m,s}}$. The normalized signals N are obtained by dividing the average signals from the sample photodiode by those from the monitor photodiode, given by

$$N_{\mathrm{x}}(\lambda, \sigma, i) = \frac{s_{\mathrm{x}}(\lambda, \sigma, i)}{s_{\mathrm{m,x}}(\lambda, \sigma, i)} \ \text{and} \tag{2.4}$$

$$N_{\mathrm{s}}(\lambda, \sigma, i, j) = \frac{s_{\mathrm{s}}(\lambda, \sigma, i, j)}{s_{\mathrm{m,s}}(\lambda, \sigma, i, j)} \ . \tag{2.5}$$

The normalized signals are used to reduce the effect of changes in the output radiant flux from the illuminator. The ratio Q_{s} of the reflectance factor of the reference standard to the normalized signal is given by

$$Q_{\mathrm{s}}(\lambda, \sigma, i, j) = \frac{R_{\mathrm{s}}(\lambda, \sigma, j)}{N_{\mathrm{s}}(\lambda, \sigma, i, j)} \ , \tag{2.6}$$

and the average of these ratios for all the reference standards is given by

$$Q_{\mathrm{s}}(\lambda, \sigma, i) = \frac{1}{m}\sum_{j=1}^{m} Q_{\mathrm{s}}(\lambda, \sigma, i, j) \ . \tag{2.7}$$

The reflectance factor R of the sample, for each scan, wavelength, and polarization, is given by

$$R_{\mathrm{x}}(\lambda,\sigma,i) = N_{\mathrm{x}}(\lambda,\sigma,i) \cdot Q_{\mathrm{s}}(\lambda,\sigma,i) \quad . \tag{2.8}$$

Averaging over polarizations, usually σ = 0° and 90° with respect to the plane of incidence, yields the reflectance factor for unpolarized incident radiant flux, given by

$$R_{\mathrm{x}}(\lambda,i) = \frac{1}{2}\left[R_{\mathrm{x}}(\lambda,0,i) + R_{\mathrm{x}}(\lambda,90,i)\right] \ . \tag{2.9}$$

The final spectral reflectance factor for a sample is obtained by averaging over all scans, n, given by

$$R_{\mathrm{x}}(\lambda) = \frac{1}{n}\sum_{i=1}^{n} R_{\mathrm{x}}(\lambda,i) \quad . \tag{2.10}$$

After the determination of the final reflectance factor, the methods specified in the next section are used to determine the color values for a specified observer and illuminant. Hereafter, for convenience, we will denote $R_{\mathrm{x}}(\lambda)$ by $R(\lambda)$.

2.2 Color Values

The color values determined by the 0:45 reflectometer consist of the Commission Internationale de l'Eclairage, (CIE) tristimulus values, chromaticity coordinates, and color-space values. The determination of each of these values is briefly discussed. Further details on the derivation and the application of these values can be found in reference [10, 11].

2.2.1 CIE Tristimulus values

The CIE tristimulus values can be determined by the integration of the spectral reflectance factor, $R(\lambda)$, over the visible wavelength range with a set of spectral weighting factors, $W(\lambda)$.

$$\begin{aligned} X &= \int_{\lambda} R(\lambda) W_x(\lambda) d\lambda , \\ Y &= \int_{\lambda} R(\lambda) W_y(\lambda) d\lambda , \\ Z &= \int_{\lambda} R(\lambda) W_z(\lambda) d\lambda , \end{aligned} \tag{2.11}$$

with

$$W_x(\lambda) = kS(\lambda)\bar{x}(\lambda)$$

$$W_y(\lambda) = kS(\lambda)\bar{y}(\lambda)$$

$$W_z(\lambda) = kS(\lambda)\bar{z}(\lambda)$$

where $S(\lambda)$ is the relative spectral power of one of the CIE standard illuminants, $\bar{x}(\lambda)$, $\bar{y}(\lambda)$ and $\bar{z}(\lambda)$ are the color matching functions of the CIE colorimetric standard observer, and k is the normalizing factor for Y equaling 100 for the perfect diffuser.

Practically, the tristimulus values are determined by a set of summations over the wavelength range. Conversion of the 2.11 equations to summations results in the following equations,

$$X = k\sum_{\lambda} R(\lambda)W(\lambda)\Delta\lambda \text{ ,} \tag{2.12}$$

$$Y = k\sum_{\lambda} R(\lambda)W(\lambda)\Delta\lambda \text{ ,}$$

$$Z = k\sum_{\lambda} R(\lambda)W(\lambda)\Delta\lambda \text{ ,}$$

with

$$k = 100 / \sum_{\lambda} S(\lambda)\bar{y}(\lambda)\Delta\lambda \text{ .}$$

The CIE defines standard tables of color matching functions and illuminant spectral power distributions for the calculation of tristimulus values [12, 13].

2.2.2 CIE Chromaticity Coordinates

The relative amounts of the tristimulus values are determined by the ratio of each value to the sum of the values. The results are referred to as the chromaticity coordinates.

$$x = X/(X+Y+Z) \tag{2.13}$$

$$y = Y/(X+Y+Z)$$

$$z = Z/(X+Y+Z) \text{ ,}$$

these coordinates satisfy the following condition

$$x + y + z = 1 \text{ .} \tag{2.14}$$

The chromaticity coordinates are generally specified by *x* and *y*, since the two known coordinates can be used to calculate the third coordinate. The two-dimensional plot of (*x*, *y*) is called the CIE 1931 chromaticity diagram.

2.2.3 CIE 1976 (*L* a* b**) Color Space

The (*x*, *y*) chromaticity coordinates specify any color of light stimuli but not the color of an object surface, which has another dimension, lightness (black to white). CIE defines two object color spaces: $L^*a^*b^*$ and $L^*u^*v^*$ [11]. In this document, $L^*a^*b^*$ is used to specify object colors, as it is most commonly used in the color community. This object color space is produced by plotting, in three dimensional coordinates, the quantities L^*, a^*, and b^* defined as follow:

$$
\begin{aligned}
L^* &= 116\left(\frac{Y}{Y_n}\right)^{1/3} - 16 \\
a^* &= 500\left[\left(\frac{X}{X_n}\right)^{1/3} - \left(\frac{Y}{Y_n}\right)^{1/3}\right] \\
b^* &= 200\left[\left(\frac{Y}{Y_n}\right)^{1/3} - \left(\frac{Z}{Z_n}\right)^{1/3}\right]
\end{aligned}
\tag{2.15}
$$

where X/X_n; Y/Y_n; $Z/Z_n > 0.01$ and X_n, Y_n, and Z_n define the tristimulus values of the reference white that is calculated from the reflectance from a perfect diffuser.

The color difference ΔE^*_{ab} between two color samples is determined from

$$\Delta E^*_{ab} = \left[(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2\right]^{1/2} \tag{2.16}$$

where $\Delta L^* = L^*_1 - L^*_2$, $\Delta a^* = a^*_1 - a^*_2$, and $\Delta b^* = b^*_1 - b^*_2$ and the subscripts 1 and 2 refer to the two samples.

3. Reference Standard

3.1 Method of Calibration

The 0:45 reflectometer measures the 0:45 spectral reflectance factor of a sample by comparing the signal from the sample and a reference standard, under the same measurement conditions, at each wavelength and two orthogonal polarizations of the incident radiant flux. The reference standards are 50.8 mm square sintered PTFE, Spectralon mounted in a 101.6 mm holder with the front of the sample parallel to the front of the sample holder. There are three reference standards denoted SP01, 02, and 03. These reference standards are also used as working standards for routine calibrations.

The reference standards are calibrated on the Spectral Tri-function Automated Reference Reflectometer (STARR) [14]. The STARR instrument is the national reference instrument for spectral reflectance measurements of spectrally neutral, non-fluorescent samples at room temperature. STARR performs absolute measurements of bi-directional reflectance on samples with widths ranging from 50 mm (2 in) to 300 mm (12 in). The measurements are all in-plane, meaning the sample normal, illumination axis, and receiver axis, all lie within the same horizontal plane.

The major components of the STARR instrument are a source, a sample holder, and a detector. The source system provides a collimated, monochromatic beam of light with a known polarization over the spectral region of 200 nm to 2500 nm. The goniometer is a monoplane gonio-instrument with a rotating sample table and a movable detector arm. The sample table and the detector arm can rotate at a constant distance independently of each other but normal to the plane of incidence. The goniometer varies the angle of incidence from 0º to 80º, and the viewing angle can be any value greater than 5º relative to the incident beam. The absolute reflectance is calculated from measurements of the incident and the reflected radiant fluxes obtained by rotating the detector arm. The receiver is attached to the goniometer and has a precision aperture, a lens, and a photodiode detector, either Si, or a cooled extended InGaAs. The sampling aperture, defined by the illumination beam, has a diameter of 17 mm and is located at the center of the calibration item. The maximum deviation of any ray within the illumination beam from the illumination angle is 0.36º. The entrance pupil of the receiver has an area of 796.7 mm^2 and is located 671.4 mm from the sampling aperture, resulting in a solid angle of collection of 0.00177 sr. The maximum deviation of any ray within the receiver beam from the viewing angle is 1.9º.

The fundamental quantity for spectral reflectance factor measurements is the bi-directional reflectance distribution function (BRDF). For a fixed linear polarization of the incident beam and incident and viewing directions in the same plane, the measurement equation for BRDF is given by

$$f_{\mathrm{r}}(\theta_{\mathrm{i}},\theta_{\mathrm{r}};\lambda;\sigma)=\frac{s_{\mathrm{r}}(\theta_{\mathrm{i}},\theta_{\mathrm{r}};\lambda;\sigma)}{s_{\mathrm{i}}(\lambda;\sigma)\cdot\Omega_{\mathrm{r}}} \tag{2.17}$$

where θ_{i} and θ_{r} are the incident and reflected angles, respectively, λ is the wavelength, σ is the polarization, s_{r} and s_{i} are the signals recorded by the detector during the measurement of the reflected radiance and incident irradiance, respectively, and Ω_{r} is the projected solid angle from the center of the area of illumination to the aperture stop of the detector. Reflectance factor, R is calculated from the BRDF by

$$R(\theta_{\mathrm{i}},\phi_{\mathrm{i}};\theta_{\mathrm{r}},\phi_{\mathrm{r}};\lambda;\sigma)=\pi\cdot f(\theta_{\mathrm{i}},\phi_{\mathrm{i}};\theta_{\mathrm{r}},\phi_{\mathrm{r}};\lambda;\sigma) \tag{2.18}$$

3.2 Uncertainty

Following the procedure for uncertainty analysis presented in Ref. [14], the relative expanded uncertainty (k=2) for the 0:45 spectral reflectance factor of Spectralon is 0.4 %. The components of uncertainly are divided into those arising from random and systematic effects. The random effects, which include signal noise, result in a relative expanded uncertainty of 0.02 %. The systematic effects, which include the wavelength uncertainty, stray light, angle of reflection, aperture stop area, and the distance from the sample to the aperture stop, result in a relative expanded uncertainty of 0.2 %.

3.3 Maintenance of Reference Standards

The reference standards are measured on STARR every year. The new reflectance factors are used in the 0:45 reflectometer measurements. The typical 0:45 spectral reflectance factor of a Spectralon reference standard is shown in Figure 3.1.

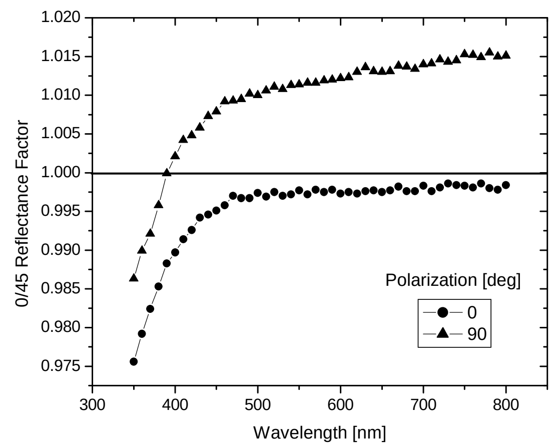


Figure 3.1 Typical 0:45 spectral reflectance factor of a Spectralon reference standard.

4. Reference 0:45 Reflectometer

4.1 Instrument Description and Properties

The 0:45 reflectometer consists of a monochromatic illuminator, sample wheel, and receiver on a vibration-isolation table and is described in details in ref. [5]. The illuminator and receiver are fixed while the sample wheel rotates holding up to 20 samples. A computer located adjacent to the instrument provides fully automated system control, data acquisition, and analysis. A schematic of the 0:45 reflectometer indicating the major components is shown in Fig 4.1.

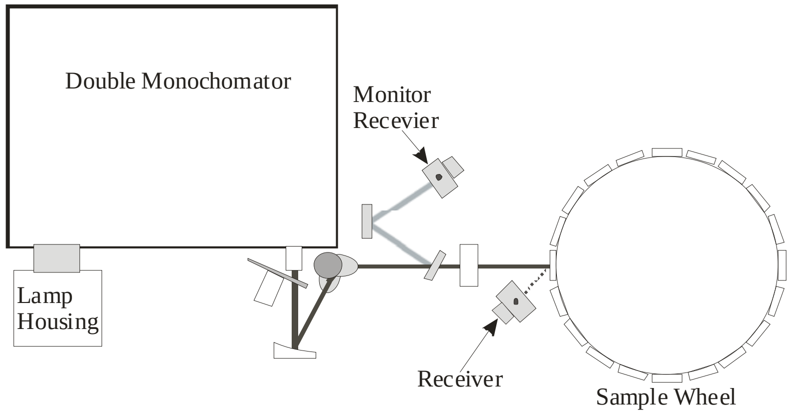


Figure 4.1 Schematic of the 0:45 reflectometer consisting of a monochromatic illuminator, sample wheel, and receivers.

The illuminator provides a monochromatic, polarized influx beam centered on the sample compartment of the sample wheel with a triangular spectral bandwidth of 5 nm at full width half maximum (FWHM). The illuminator consists of a dual-source illuminator, filter wheel, double monochromator, telecentric aperture, light chopper, ellipsoidal and flat mirrors, silica window, monitor diode, and polarizer.

The monochromator dual illuminator housing holds a 150 W Xe arc lamp and a 100 W quartz-tungsten-halogen (QTH) incandescent lamp. The sources are selected by rotating a mirror. In general, the Xe lamp is used for wavelengths ≤ 460 nm and the QTH lamp is used for wavelengths > 460 nm. The filter wheel has four long-pass filters which are used for order-sorting to eliminate higher-order wavelengths from passing through the monochromator and is located between the source and entrance slit of the monochromator.

The double additive monochromator has a focal length of half meter and f/# of 7.3. The gratings are 110 mm square, 600 grooves/mm, and are blazed at 550 nm. The mirrors and gratings are coated with aluminum (Al) on a quartz substrate with an over-coating of magnesium fluoride (MgF_2). The focal length of the exit mirror is 546 mm giving a mirror magnification ratio of 1.1. There is a slit height mask of 4 mm on the exit slit cemented to the inside of the slit assembly. A telecentric aperture of diameter 7.23 mm is attached to the monochromator exit slit assembly at 75 mm ± 0.3 mm from the exit slit plane and defines the convergence angle to be ± 0.95°. In a telecentric configuration, the aperture stop is placed at the focal point of the lens therefore the central ray of each bundle is parallel to the lens axis providing uniform illumination on the sample. An optical light chopper is placed after the telecentric aperture. The chopper is used to square-wave modulate the intensity of the optical signal at a stable frequency which can be amplified easily.

A 15° off-axis ellipsoidal mirror made of Al and Ni plated with a protective layer of MgF_2, surface roughness of 2 nm, f_1 = 300 mm, and f_2 = 900 mm is used to relay the exit slit of the monochromator to the sample plane. This mirror has a 177.8 mm focal length mirror with a 3 times magnification which produces a 10 mm x 12 mm rectangular illumination area on the sample. A periscope follows the ellipsoidal mirror to steer the beam for alignment and to compensate for the difference in height between the exit slit of the monochromator and the sample plane. The polarizer is a Glan-Thompson polarizing prism with an extinction ratio of 1×10^{-6} at $\lambda = 633$ nm and is used to perform measurements for polarizations of the incident beam both parallel and perpendicular to the plane of incidence. The monitor diode is the same type as the signal diode described below. The purpose is to monitor the influx beam to correct for drift in the output of the instrument illuminator. Figure 4.2 shows a top view of the components and optical path of the illuminator.

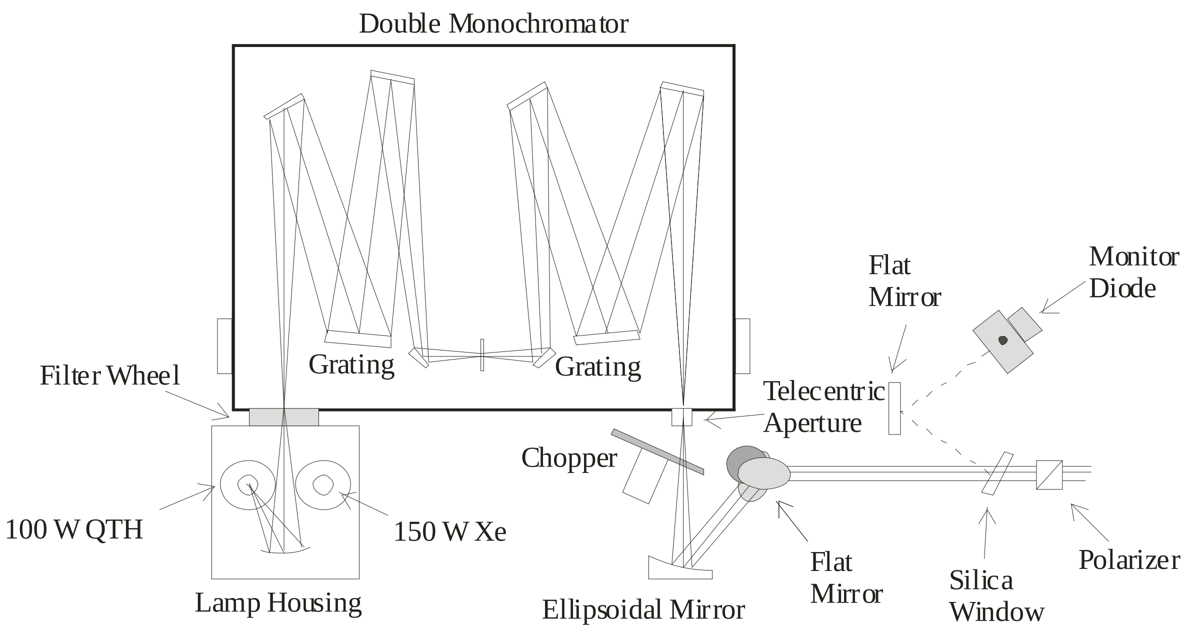


Figure 4.2 Top view of the components and optical path of the illuminator.

Motions of the monochromator components including the grating, port selection, and slit width, filter wheel, and source selector are driven by precision stepper motors. The grating position is read by an absolute rotary encoder attached to the end of the grating lead screw.

The sample wheel is custom-made and is mounted on a computer control rotation stage. The wheel is 81 cm in diameter, fabricated from one piece of aluminum, and has 20 sample compartments. Each sample compartment can be individually aligned. Samples with widths from 3 cm to 10 cm and heights from 3 cm to 20 cm can be accommodated.

The receiver measures the efflux beam from the sample at an angle of 45° and consists of a bi-convex lens, a telecentric aperture stop, and a Si photodiode mounted in a tube. The receiver aperture is 3.55 mm in diameter and is located 3.5 mm from the receiver. The telecentric aperture is sized to provide a receiver half subtended angle of ±

1.36°, to closely match the geometry of STARR. The detector is underfilled with the image of the illumination area at an exitance of 45° to the sample plane. A schematic of the optical path of the receiver is shown in Fig. 4.3. A summary of the geometrical specifications of the 0:45 reflectometer is given in Table 4.1.

The receiver lens is an achromat mounted with an optimized meniscus lens with an effective focal length of 70.5 mm and coated for low reflectance in the visible wavelength region. The receiver optical detector is a Si photodiode with UV to visible sensitivity and suppressed IR sensitivity and an active area of 10 mm x 10 mm. The current from the Si photodiode is converted to voltage by a transimpedance amplifier and measured with a lock-in amplifier which auto-ranges. The signal from the test sample is normalized to the signal from the reference standard. A signal proportional to the reflected radiant flux is measured at each wavelength and each sample for one polarization. Then, the polarization is rotated and the measurements are repeated.

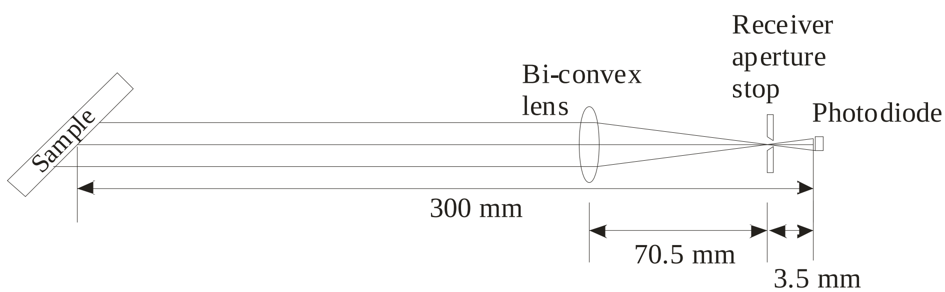


Figure 4.3 Schematic of the optical path of the receiver.

Table 4.1 Geometrical specifications of 0:45 reflectometer

	Illuminator	***Receiver***
Type of geometry	Directional	Directional (uniplanar)
Direction of axis	0° ± 0.1°	45° ± 0.1°
Area	10 mm by 12 mm	20 mm by 24 mm
Cone half-angle	0.30°	1.36°

4.2 Characterization of Instrument

The line spectral function (LSF) was measured by scanning several lines of emission lamps with variable entrance and exit slit widths. An example is shown in Fig. 4.4 of the 546.074 nm line of an Hg emission lamp with variable entrance and exit slit widths. An entrance slit width of 3.01 mm, exit slit width of 3.31 mm, and center slit width of 4 mm, results in a triangular spectral bandwidth at FWHM of 5 nm.

The stray-light rejection level was measured using a multimode Ar^+ laser illuminating an integrating sphere at the front entrance slit. The bandwidth was set to 5 nm with no polarizer in the beam path and a 22.5° mirror placed in one of the sample compartments. The stray-light rejection level was determined to be 1×10^{-3} 5 nm away from the set wavelength and 1×10^{-6} 15 nm away from the set wavelength.

The wavelength scale was calibrated using a 22.5° mirror at the sample position, the polarizer was removed from the beam path, and an integrating sphere illuminated with pen-ray lamps was placed at the front entrance port. The emission lamps and corresponding lines are listed in Table 4.2. These emission lines were selected for their signal strength and separation from other emission lines. The front entrance slit was set to a width of 1.73 mm, the front exit slit was set to 1.9 mm, and the center slit was set to 4 mm. Wavelength scale calibration of the monochromator relates the motor step of the grating drive to wavelength. The calibration consists of scanning a set of emission lines, calculating the motor step centroids of the lines, and fitting the wavelengths of the lines to the centroids. Single fits were able to reproduce the wavelengths of the lines to within 0.01 nm. However, the motor step centroids changed with each scan, and these changes were within 0.05 nm. Therefore, the standard uncertainty in wavelength scale is assigned to be $u(\lambda_i) = 0.05$ nm at all wavelengths. This provides a conservative estimate of the wavelength uncertainty without considering further details about possible wavelength dependencies. A summary of the spectral specifications of the illuminator is given in Table 4.3.

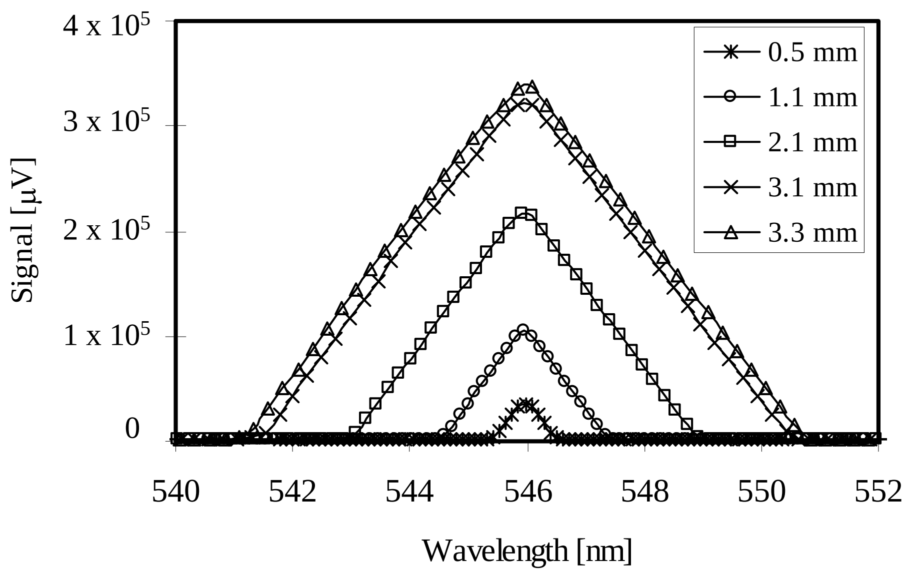


Figure 4.4 Spectral line spread function measured by scanning over the 546.074 nm Hg lamp emission line using variable exit slit widths as listed in the legend. The entrance slit width was 0.909 of the exit slit width and the center slit width was 4 mm.

Table 4.2 Sources and wavelength of emission lines used for the wavelength calibration.

Source	Wavelength [nm]
Hg	435.834
Hg	546.074
Ne	692.947
Ar	763.510

Table 4.3 Spectral specifications of 0:45 illuminator

Property	**Value**
Wavelength Range	380 nm to 780 nm/ 5nm interval
Spectral Bandwidth	5 nm, triangular
Stray-light Rejection	less than 1.5×10^{-6}
Wavelength Uncertainty	0.05 nm (standard uncertainty)
Polarization	0º (parallel to plane of illumination) 90º (perpendicular to plane of illumination)

Each sample compartment was aligned by placing a mirror and adjusting the degrees of freedom so that the reflection was retro-reflected. Differences in the angles of illumination and viewing are less than 0.04°, based upon the angular alignment of each sample position. In addition, a set of color tiles was measured multiple times in random sample compartments of the sample wheel and no changes were found correlated with the sample compartments.

The signals are assumed to be directly proportional to the radiant fluxes reflected by the sample and reference standard. The measured signal levels depend on the sample being measured. For dark colored samples such as black or deep gray the reflected flux is lower than for the reference standard. Therefore, several sensitivity ranges of the lock-in-amplifiers are required to cover the dynamic range. The linearity of the photodiode-amplifier-lock-in-amplifier combination was measured at the sensitivity ranges used during data acquisition. The signal levels at the detector were adjusted by scanning the wavelength of the monochromator to yield radiant flux levels at the different sensitivity ranges used in the lock-in-amplifier during measurements. The measured relative responsivity of the photodiode-amplifier combination is linear within 0.2 % for the sensitivity ranges of 50 µV to 20 mV.

4.3 Instrument Validation

The purpose of validation is to ensure proper operation of the 0:45 Reflectometer and is accomplished by repeated measurements of check standards. These measurements over time provide the control charts for the instrument to track its performance. The validation of the instrument includes measurements of reference, check, and comparison standards.

The reference standards are measured on STARR every year for the measurement geometry of 0:45 and the wavelength range of 380 nm to 780 nm at 5 nm increments. The reference standards are 50.8 mm square Spectralon mounted in a 101.6 mm square holder with the front of the Spectralon parallel to the front of the sample holder.

The check standards for the 0:45 reflectometer are measured every year, or after significant changes to the instrument, to verify proper operation of the 0:45 reflectometer. The check standards are all fourteen BCRA Series II tiles, serial number NISTCS-1. The CIE Lab color space values are determined and recorded in a spreadsheet to distinguish any changes in the measured values outside of the expanded uncertainty (k = 2). The 0:45 spectral reflectance factors of selected check standards are measured during each calibration. The selected check standards are the cyan, deep grey and orange tiles of set NIST CS-1. The 0:45 spectral reflectance factors of the three selected check standards are shown in Fig. 4.5. The measured spectral reflectance factors of the tiles should be within the expanded uncertainties of the 0:45 reflectometer. Control charts are maintained for measured L, a, and b values of the check standard. Figure 4.6 is a control chart for the measured L for the cyan tile. The lines represent the tolerance condition which is based on a 95 % confidence interval of the instrument repeatability.

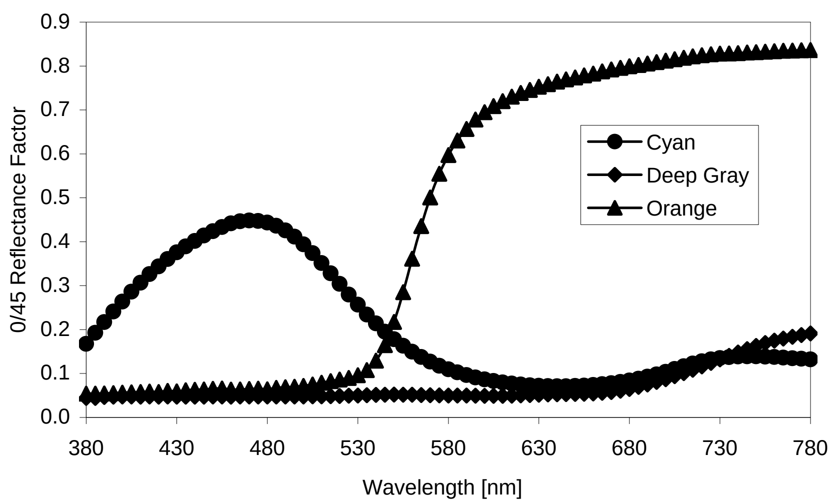


Figure 4.5 Typical 0:45 spectral reflectance factors of cyan, deep gray, and orange check standards.

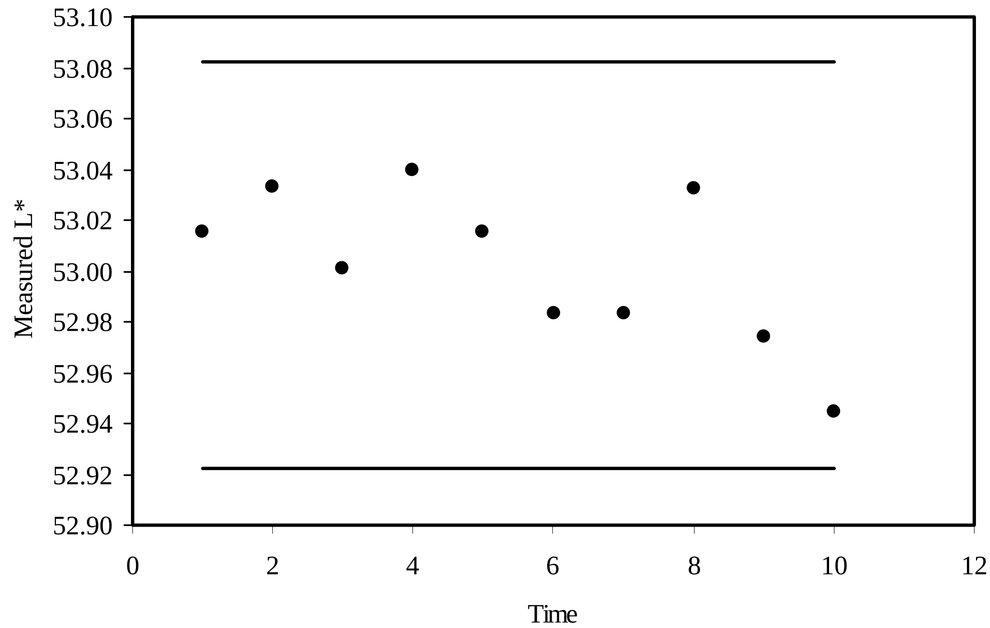


Figure 4.6 Control chart of the measured *L** for the cyan tile. The solid lines represent the tolerance condition.

The comparison standards are measured as needed on both the 0:45 reflectometer and on STARR to verify equivalence between the two instruments for neutral colors. The comparison standards are five neutral, matte BCRA Series II tiles, serial number NS-1, listed in Table 4.4.

Table 4.4 Comparison Standards

Sample
White
70 % Grey
Mid Grey
40 % Grey
Black

The five tiles are placed in the sample compartments of the 0:45 reflectometer along with the reference standards. The spectral reflectance factors for each tile are determined and each value is compared to the values obtained with STARR. The spectral reflectance factors should be within the combined expanded uncertainties due to random effects.

4.4 Calibration Services

The 0:45 measurements are available at cost on submitted samples or as a set of calibrated BCRA Series II color tiles available for purchase. A preliminary discussion with NIST staff is required before the samples are submitted.

Upon receipt of submitted samples, the samples are inspected and the condition is noted. Submitted samples that do not meet the minimum requirements listed in Table 4.5 require additional arrangements before acceptance. The samples will not be cleaned with the exception of dust that can be removed with an air bulb blower. The samples are kept in the original measurement container provided by the customer, and powder free gloves are used while handling the sample to prevent contamination.

Table 4.5 Acceptance criteria for 0:45 test samples

Physical Damage	Sample should be undamaged in the measurement area (No major scratches, chips, etc.)
Uniformity	The samples should be of uniform appearance in the measurement area (i.e. smooth, no stains and no fingerprints).
Fluorescence	Samples should not exhibit fluorescence upon radiation in the measurement spectrum (360 nm to 800 nm)
Cleanliness	The measurement surface of the sample should be clean. Foreign contaminants other than light dust will not be removed from the sample surface

The availability of BCRA Series II color tiles from NIST is dependent on the availability from the supplier. The color tile set consists of fourteen BCRA glossy color tiles manufactured by CERAM Research, 10 cm square. The set is divided in a wooden box containing twelve colored tiles and a twin box containing a black and a white tile. Each tile in the set is identified by its color designation.

An example of the calibration report for the set of BCRA Series II tiles is provided for reference in Appendix A of this document. This report provides a description of the calibration items, the calibration method, results, and general information on the calibration.

5. Uncertainty Analysis

The purpose of the 0:45 reflectometer is to provide calibrations of color standards of the highest possible quality to establish traceability which requires an estimate of the uncertainty [15]. Therefore the uncertainties in the color standard samples provided by the NIST 0:45 reflectometer are carefully determined following international accepted protocols describe in the *ISO Guide to the Expression of Uncertainty in Measurement* [16]. Recent publications have applied the principles of this Guide to uncertainty analysis for colorimetry, emphasizing the treatment of correlation [17,18]

The sources of uncertainty associated with the 0:45 reflectometer were identified from the characterization of the instrument [5]. The components of uncertainties were characterized and analyzed in [19, 20]. The procedure for determining these uncertainties follows the approach given in [21], which presents a systematic, analytical method for calculating uncertainties. Two key points are emphasized in this method. First, the measurement equation, which relates the measured signals to the reflectance factor, is the starting point for the analysis (this has been developed in section 2 of this work). Since ratios of signals are present in the measurement equation, the spectral properties of the reference reflectance reflectometer are required. Second, the effects of correlations both between signals at the same wavelength and between reflectance factors at different wavelengths must be included in the analysis. Once the uncertainties of all components in these measurements have been established, the uncertainties in the other values may be determined by the propagation of uncertainties.

The systematic, analytical method for calculating uncertainties presented in reference [19] provides a step-by-step procedure for analyzing uncertainties, and this procedure is followed here. The steps are

1. Identify all independent sources of uncertainty.
2. Assign standard uncertainties to these sources of uncertainty.
3. Calculate the standard uncertainty (called uncertainty contribution) in spectral reflectance factor, $u(R(\lambda_i))$, for each source of uncertainty, using the measurement equation and taking any correlations between signals at the same wavelength into account.
4. Calculate the correlation coefficient between spectral reflectance factors at different wavelengths, $r(R(\lambda_i), R(\lambda_j))$, for each source of uncertainty.
5. Calculate the sensitivity coefficient for each color space value Γ with respect to $R(\lambda_i)$.
6. Calculate the uncertainty contribution in each color space value, $u(\Gamma)$, using the results from steps 3 and 4 for each source of uncertainty.
7. Calculate the combined standard uncertainty, u_c, in each color space value according to the uncertainty propagation principle.
8. Calculate expanded uncertainty, U, with a coverage factor ($k = 2$).

5.1 Sources of Uncertainty

The sources of uncertainty associated with the 0:45 reflectometer are mainly the signals from the sample and reference standard, the wavelength of the monochromator, bandpass of the monochromator, and the reflectance factor of the reference standard. The uncertainties in L^*, a^*, and b^* from these sources of uncertainty are evaluated for a set of color tiles, which are available as calibrated standards from NIST. Therefore, in the following the terms sample and color tile are synonymous.

Uncertainties in the L^*, a^*, and b^* values caused by random effects, primarily signal noise in both the sample and monitor receivers, are evaluated by Type A methods and are given by the standard deviations, u_1, of the values from ten repeat measurements.

Uncertainties in the signals caused by systematic effects are evaluated by Type B methods and are non-linearity of the signal from the sample relative to the signal from the reference standard, and the effect of stray-light on both signals. Mis-alignment of the specimen is a possible source of uncertainty and is a result of a difference in angle or location, with respect to the reference plane, between the specimen and reference standard. Differences in the angles of illumination and viewing are less than 0.04°, based upon the angular alignment of each sample position. The changes in reflectance factors resulting from these differences were evaluated for each color tile using the reference reflectometer, and found to be negligible. Because the receiver is a telecentric optical system, and the size of the sampling aperture is less than the field-of-view of the receiver at the reference plane, differences in location between the specimen and reference standard with respect to the reference plane have no effect on the measured reflectance factor of a uniform sample.

The signals are assumed to be directly proportional to the radiant fluxes reflected by the sample and reference standard. However, non-linearity of the detector results in the ratio of the signals not being equal to the ratio of the reflected fluxes. Non-linearity arises both within the ranges of the current-to-voltage and lock-in amplifiers and between ranges of the lock-in amplifier. The relative standard uncertainty in the signal from the sample due to non-linearity is

$$\frac{u_1(S_x(\lambda_i,\sigma))}{S_x(\lambda_i,\sigma)} = 0.002 \tag{5.1}$$

Stray-light is radiant flux that reaches the detector at wavelengths outside the nominal spectral bandwidth of the instrument, which contributes to the signal. This contribution depends upon the spectral distribution of the illuminator, the spectral reflectance of both the sample and reference standard, and the responsivity of the receiver. The stray-light rejection of the monochromator is less than 10^{-6} at wavelengths 10 nm and larger from the set wavelength, and 10^{-3} at wavelengths 5 nm from the set wavelength. Therefore, the estimated error in the signals due to stray-light is given by

$$\varepsilon\left(s(\lambda_i,\sigma)\right) = \sum_{\lambda'} s(\lambda',\sigma)\cdot 10^{-6} + 10^{-3}\left[s(\lambda_i - 5,\sigma) + s(\lambda_i + 5,\sigma)\right] \tag{5.2}$$

where s is the signal from either the sample or reference standard and the summation is over all wavelengths from 350 nm to 1100 nm for the source used at wavelength λ_i, excluding those at wavelengths of λ_i – 5 nm, λ_i, and λ_i + 5 nm.

The wavelength calibration of the monochromator was discussed in Section 4.2 and resulted in a standard uncertainty in wavelength of $u(\lambda_i)$ = 0.05 nm at all wavelengths.

The bandpass of the monochromator can cause errors when the spectral reflectance factor curve is not linear within the full-bandwidth of the bandpass, and can cause significant errors where spectral reflectance factor curves change rapidly, e.g., for saturated color samples. The measured spectral reflectance factor is a convolution of the true reflectance factor and the normalized bandpass function. At each wavelength point, measured reflectance factor $R_{\mathrm{m}}(\lambda_0)$ is calculated as a product of the true spectral reflectance factor $R(\lambda)$ and the normalized bandpass function $z_0(\lambda)$, thus,

$$R_{\mathrm{m}}(\lambda_0) = \int_{\lambda} R(\lambda_0 - \lambda) \cdot z(\lambda_0 - \lambda)\,\mathrm{d}\lambda \qquad \text{with} \qquad \int_{\lambda} z(\lambda) = 1. \tag{5.3}$$

An example of the bandpass function $z_0(\lambda)$ is shown in Fig. 5.1.

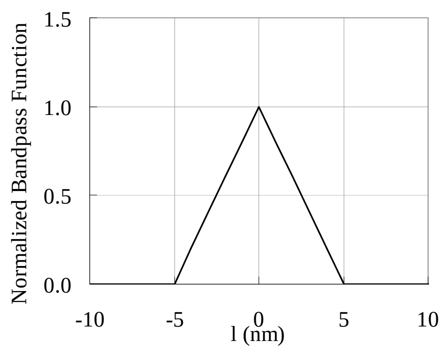


Fig. 5.1 An example of a bandpass function $z_0(\lambda)$.

To estimate this error without knowing the true reflectance factor $R(\lambda)$, the measured data is used as $R(\lambda)$ for an approximation. The spectral reflectance factor data is first interpolated to 1 nm interval, and the z(λ) function (normally a triangular function) also prepared at 1 nm intervals, normalized so that the sum of all z(λ) values is equal to 1, then a sum-product calculation is performed as given in Eq. (5.3). The relative error due to the bandpass can be evaluated by looking at the difference between $R_{\mathrm{m}}(\lambda)$ and $R(\lambda)$.

$$\varepsilon_{\mathrm{B,rel}}(\lambda) = \frac{R_{\mathrm{m}}(\lambda) - R(\lambda)}{R(\lambda)} \tag{5.4}$$

In substitution measurements, this error tends to be cancelled out if the sample and reference standard have similar spectral reflectance factor curves. In this case, the relative error for the sample $\varepsilon_{\mathrm{B,rel,sample}}(\lambda)$ and for the reference standard $\varepsilon_{\mathrm{B,rel,std}}(\lambda)$ can be calculated, respectively, and the substitution error $\varepsilon_{\mathrm{B,sub}}(\lambda)$ in the measured test sample is given by

$$\varepsilon_{\mathrm{B,sub}}(\lambda) = \varepsilon_{\mathrm{B,rel,sample}}(\lambda) - \varepsilon_{\mathrm{B,rel,std}}(\lambda) \tag{5.5}$$

An example of the calculation of bandpass error for a yellow BCRA tile for a triangular bandpass of 5 nm (FWHM) is shown in Fig. 5.2.

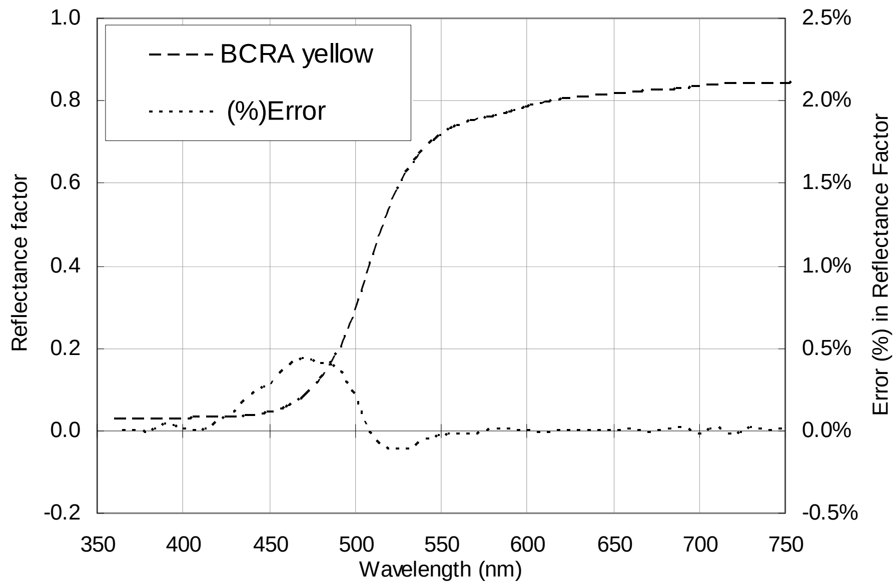


Fig. 5.2 An example of the error due to a 5 nm (FWHM) triangular bandpass of the monochromator for the measurement of a yellow BCRA tile. The corresponding error in color difference is ΔE^*_{ab} = 0.09.

The error in a color quantity Γ (such as L^*, a^*, b^*) is given by calculating the color quantity value from $R_m(\lambda)$ and $R(\lambda)$,

$$\varepsilon_{\mathrm{B,sub}}(\Gamma) = \Gamma(R_m(\lambda)) - \Gamma(R(\lambda)) \tag{5.6}$$

If this error is not corrected, this estimated error is converted to a standard uncertainty by

$$u_2(\Gamma) = \varepsilon_{\mathrm{B,sub}}(\Gamma)/\sqrt{3} \tag{5.7}$$

The calculation presented above is only for estimation of error. For correction of bandpass errors, other methods [22, 23] are available.

The relative standard uncertainties due to random and systematic effects during the calibration of the reference standards with STARR are

$$\frac{u_3(R_s(\lambda_i,\sigma))}{R_s(\lambda_i,\sigma)} = 0.0002 \text{ and} \tag{5.8}$$

$$\frac{u_4(R_s(\lambda_i,\sigma))}{R_s(\lambda_i,\sigma)} = 0.002 \ , \tag{5.9}$$

respectively, and are both evaluated using Type B methods for the uncertainty analysis of the 0:45 reflectometer.

5.2 Uncertainty and Correlation of *R*(*λ*)

Determining the standard uncertainty $u(R(\lambda_i))$ for each source of uncertainty caused by systematic effects uses Eqs. (2.1) and (2.2), which relate the reflectance factor of the sample to the signals and the reflectance factor of the reference standard, and the reflectance factor for unpolarized incident radiant flux to the reflectance factors when the incident radiant flux is polarized. Beginning with polarized incident radiant flux, from Eq. 2.1, the standard uncertainty due to uncertainties in the signals is given by

$$\frac{u^2(R(\lambda_i,\sigma))}{R^2(\lambda_i,\sigma)} = \frac{u^2(s_\mathrm{x}(\lambda_i,\sigma))}{s_\mathrm{x}^2(\lambda_i,\sigma)} + \frac{u^2(s_\mathrm{s}(\lambda_i,\sigma))}{s_\mathrm{s}^2(\lambda_i,\sigma)} - 2\frac{u(s_\mathrm{x}(\lambda_i,\sigma))}{s_\mathrm{x}(\lambda_i,\sigma)}\frac{u(s_s(\lambda_i,\sigma))}{s_s(\lambda_i,\sigma)} r(s_\mathrm{x}(\lambda_i,\sigma), s_s(\lambda_i,\sigma)) \tag{5.10}$$

For non-linearity of the signal from the sample, $u(s_\mathrm{s}(\lambda_i, \sigma) = 0$ and Eq. 5.10 reduces to

$$\frac{u_5(R(\lambda_i,\sigma))}{R(\lambda_i,\sigma)} = \frac{u_4(s_x(\lambda_i,\sigma))}{s_x(\lambda_i,\sigma)} \ . \tag{5.11}$$

For stray-light effects on both signals, the correlation coefficient $r(s_\mathrm{x}(\lambda_i, \sigma), s_\mathrm{s}(\lambda_i, \sigma)) = 1$ and Eq. 5.10 reduces to

$$\frac{u_6(R(\lambda_i,\sigma))}{R(\lambda_i,\sigma)} = \left[\frac{u_5(s_x(\lambda_i,\sigma))}{s_x(\lambda_i,\sigma)} - \frac{u_5(s_\mathrm{s}(\lambda_i,\sigma))}{s_s(\lambda_i,\sigma)}\right] \ . \tag{5.12}$$

The uncertainty in R due to the wavelength uncertainty is also fully correlated between the signals from the sample and the reference standard, and the relative standard uncertainty is given by

$$\frac{u_7(R(\lambda_i,\sigma))}{R_s(\lambda_i,\sigma)} = \left|\frac{\partial\left(S_x(\lambda_i,\sigma) / S_s(\lambda_i,\sigma)\right)}{\partial\lambda}\right| \cdot u(\lambda) \ . \tag{5.13}$$

Proceeding to unpolarized incident radiant flux, from Eq. 2.2, the reference standard uncertainty is given by

$$u^2\big(R(\lambda_i)\big) = \frac{1}{4}u^2\big(R(\lambda_i,0°)\big) + \frac{1}{4}u^2\big(R(\lambda_i,90°)\big) + \frac{1}{2}u\big(R(\lambda_i,0°)\big)u\big(R(\lambda_i,90°)\big)\cdot r\big(R(\lambda_i,0°), R(\lambda_i,90°)\big) \tag{5.14}$$

Assuming the sources of uncertainty are completely correlated between polarizations, so $r(R(\lambda_i,0°), R(\lambda_i,90°)) = 1$ and Eq. 5.14 reduces to

$$u\big(R(\lambda_i)\big) = \frac{1}{2}\big[u\big(R(\lambda_i,0°)\big) + u\big(R(\lambda_i,90°)\big)\big] \ . \tag{5.15}$$

From Eq. 5.10, the correlation coefficients $r(R(\lambda_i), R(\lambda_j))$ between reflectance factors at wavelengths λ_i and λ_j are needed for the calculation of uncertainties in L^*, a^*, and b^*. For uncertainties caused by non-linearity of the signal, the correlation coefficient is one, while for uncertainties caused by stray-light the correlation coefficient is

$$r(R(\lambda_i), R(\lambda_j)) = \mathrm{sgn}\left(\frac{1}{s_x(\lambda_i)} - \frac{1}{s_\mathrm{s}(\lambda_i)}\right)\cdot \mathrm{sgn}\left(\frac{1}{s_x(\lambda_j)} - \frac{1}{s_\mathrm{s}(\lambda_j)}\right) \ . \tag{5.16}$$

However, since $s_\mathrm{s} > s_\mathrm{x}$ at all wavelengths for the reference standard used, the correlation coefficient is one. For uncertainties caused by wavelength, which are treated as constant in magnitude and sign at all wavelengths, the correlation coefficient is

$$r(R(\lambda_i), R(\lambda_j)) = \mathrm{sgn}\left(\frac{\partial\left(s_\mathrm{x}(\lambda_i)\big/ s_\mathrm{s}(\lambda_i)\right)}{\partial\lambda}\right)\cdot \mathrm{sgn}\left(\frac{\partial\left(s_\mathrm{x}(\lambda_j)\big/ s_\mathrm{s}(\lambda_j)\right)}{\partial\lambda}\right) , \tag{5.17}$$

while for uncertainties caused by the reflectance factor of the reference standard, the correlation coefficient is zero for those caused by random effects and is assumed to be one for those caused by systematic effects.

5.3 Uncertainties in *L**, *a**, and *b**

The uncertainties in L^*, a^*, and b^* are obtained by propagating the uncertainties in $R(\lambda_i)$ using

$$u^2(\Gamma) = \sum_{i=1}^{m}\left(\frac{\partial\Gamma}{\partial R(\lambda_i)}\right)^2 u^2(R(\lambda_i)) + 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left(\frac{\partial\Gamma}{\partial R(\lambda_i)}\right)\left(\frac{\partial\Gamma}{\partial R(\lambda_j)}\right)\cdot r(R(\lambda_i), R(\lambda_j))\cdot u(R(\lambda_i))\cdot u(R(\lambda_j)) \tag{5.18}$$

where Γ represents any of the color space values, $u(R(\lambda_i))$ is the standard uncertainty of the reflectance factor at wavelength λ_i, and $r(R(\lambda_i), R(\lambda_j))$ is the correlation coefficient between reflectance factors at different wavelengths. The sensitivity coefficients are given by

$$\frac{\partial L^*}{\partial R(\lambda_i)} = \frac{116}{3}\left(\frac{1}{Y^2 Y_{\mathrm{n}}}\right)^{1/3} \cdot W_y(\lambda_i) \ , \tag{5.19}$$

$$\frac{\partial a^*}{\partial R(\lambda_i)} = \left[\frac{500}{3}\left(\frac{1}{X^2 X_{\mathrm{n}}}\right)^{1/3}\right] \cdot W_x(\lambda_i) - \left[\frac{500}{3}\left(\frac{1}{Y^2 Y_{\mathrm{n}}}\right)^{1/3}\right] \cdot W_y(\lambda_i) \ , \text{ and} \tag{5.20}$$

$$\frac{\partial b^*}{\partial R(\lambda_i)} = \left[\frac{200}{3}\left(\frac{1}{Y^2 Y_{\mathrm{n}}}\right)^{1/3}\right] \cdot W_y(\lambda_i) - \left[\frac{200}{3}\left(\frac{1}{Z^2 Z_{\mathrm{n}}}\right)^{1/3}\right] \cdot W_z(\lambda_i) \ . \tag{5.21}$$

The uncertainties in L^*, a^*, and b^* for a set of color tiles available from NIST as calibrated standards were calculated for each source of uncertainty for CIE Standard Illuminant D65 and the 1931 CIE 2° Standard Observer. The uncertainties caused by random effects were calculated from the standard deviations of L^*, a^*, and b^* from repeat measurements of each color tile. Therefore, only systematic effects are considered for other sources of uncertainty. The results are given in Table 5.1 for a representative set of color tiles. The expanded uncertainty U is the root-sum-square of the standard uncertainties from all the sources, multiplied by a coverage factor $k = 2$. The uncertainties for the CIE 1964 Standard Observer are similar to those in Table 5.1. Except for the uncertainties caused by repeatability, which change slightly with each set of measurements of a color tile set, the other uncertainties are those listed in the calibration report that accompanies a set of calibrated color tiles.

Color difference and combined color uncertainty are two distinct yet related concepts in color space. The following discussion is meant to provide a simple approach on the relationship between the two; a full analysis is beyond the scope of this paper. Color difference ΔE^*_{ab} in the CIELAB color space applies to comparisons between the color space values of two different specimens, or to a single specimen measured by two different instruments. The color difference is given by

$$\Delta E^*_{\mathrm{ab}} = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2} \ , \tag{5.22}$$

where ΔL^*, Δa^*, and Δb^* are the differences in color space values. Combined color uncertainty ΔE applies to a single measurement on a single specimen, and is given by

$$\Delta E = \sqrt{u^2(L^*) + u^2(a^*) + u^2(b^*)} \ . \tag{5.23}$$

The combined color uncertainty assists with interpreting a color difference. Let ΔE_1 and ΔE_2 be the combined color uncertainties of two different specimens, or a single specimen measured by two different instruments. If the relationship $\Delta E^*_{ab} < \sqrt{(\Delta E_1)^2 + (\Delta E_2)^2}$ is valid, then the color space values agree within the limits imposed by the uncertainties. If the relationship is not valid, then the color space values disagree. Values of ΔE for all the color tiles are given in Table 5.1. Note that the expanded, combined color uncertainties are all less than 0.5, indicating that the design goal for the NIST 0:45 reflectometer was met for all the standard color tiles.

Since tables of numbers are often difficult to easily interpret, the uncertainties for selected color tiles (those used in Ref. [19]) are presented in Fig. 5.3. The two most significant differences between the previous analysis presented in ref. [19] and the one presented here are the inclusion of the polarization of the incident radiant flux and evaluating the effects of signal noise from repeat measurements rather than assuming a constant noise of 0.1 % for all signals. Other differences are an uncertainty from an non-linearity of the signal of 0.2 % rather than 0.1 %, a more sophisticated calculation of the contribution to the signals from stray-light rejection level by including signals from both sources over the entire wavelength range of responsivity of the silicon detector, and an improved wavelength uncertainty of 0.05 nm rather than 0.1 nm. The standard uncertainties of the reference standard remained unchanged.

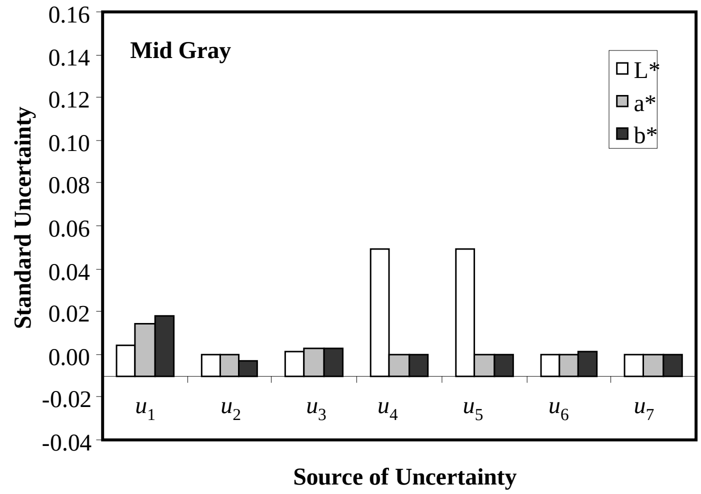
Several generalities and conclusions can be drawn from Table 5.1 and Figure 5.3. For the neutral color tiles (black, deep gray, mid gray, diff gray, pale gray, and white), there is negligible uncertainty due to stray-light and wavelength since the spectral shapes of the reflectance factors of these samples are similar to that of the reference standard. The uncertainties due to signal non-linearity affect only the uncertainty in L^* and are generally directly proportional to L^*, whereas uncertainties due to repeatability affect the uncertainties in L^*, a^*, and b^* and are generally inversely proportional to L^*.

For the colored color tiles (deep pink, red, orange, yellow, green, diff green, cyan, and deep blue), uncertainties from all the sources contribute to the combined uncertainties in L^*, a^*, and b^*. Uncertainties due to repeatability affect all the color space values, and are roughly directly proportional to L^*, as are uncertainties due to signal non-linearity. Uncertainties due to signal stray-light depend on the spectral shape of the reflectance factor, and are largest for those colors with rapid changes from low to high reflectance factor (red, orange, and yellow). Overall, those color tiles whose reflectance factors have a spectral shape similar to that of the reference standard have the lowest uncertainties in color space values.

Table 5.1 Standard, u, and expanded (k = 2), U, uncertainties of the CIELAB values for each source of uncertainty for CIE Illuminant D65 and the CIE 1931 Standard Observer and the indicated color tiles. The standard uncertainties are u_1 – repeatability, u_2 – bandpass of the monochromator, u_3 – random effects from the calibration of the reference standard, u_4 – systematic effects from the calibration of the reference standard, u_5 – non-linearity of the signals due to non-linearity of the detectors, u_6 – stray light effects, and u_7 – wavelength of the monochromator.

Color Tile	Value		Standard Uncertainty							u_c	U
			u_1	u_2	u_3	u_4	u_5	u_6	u_7		
Black	L^*	5.63	0.025	0.000	0.000	0.014	0.014	0.005	0.000	0.03	0.06
	a^*	-1.36	0.043	0.002	0.001	0.001	0.001	0.005	0.001	0.04	0.09
	b^*	0.05	0.060	-0.001	0.001	0.000	0.000	0.021	0.000	0.06	0.13
	ΔE		0.078	0.002	0.001	0.014	0.014	0.022	0.001	0.08	0.17
Deep Gray	L^*	26.97	0.005	0.000	0.001	0.029	0.029	0.004	0.000	0.04	0.08
	a^*	-0.14	0.007	0.003	0.002	0.000	0.000	0.003	0.000	0.01	0.02
	b^*	1.33	0.032	-0.003	0.001	0.001	0.001	0.017	0.001	0.04	0.07
	ΔE		0.033	0.004	0.002	0.029	0.029	0.018	0.001	0.06	0.11
Mid Gray	L^*	57.63	0.004	0.000	0.001	0.049	0.049	0.000	0.000	0.07	0.14
	a^*	-0.15	0.014	0.000	0.003	0.000	0.000	0.000	0.000	0.01	0.03
	b^*	0.55	0.018	-0.003	0.003	0.000	0.000	0.001	0.000	0.02	0.04
	ΔE		0.023	0.003	0.004	0.049	0.049	0.001	0.001	0.07	0.15
Diff Gray	L^*	58.21	0.003	0.000	0.001	0.049	0.049	0.000	0.000	0.07	0.14
	a^*	-2.50	0.007	0.002	0.003	0.002	0.002	0.000	0.001	0.01	0.02
	b^*	2.41	0.011	-0.004	0.003	0.002	0.002	0.001	0.004	0.01	0.03
	ΔE		0.013	0.004	0.004	0.050	0.050	0.001	0.005	0.07	0.14
Pale Gray	L^*	83.43	0.002	0.000	0.001	0.066	0.066	0.000	0.000	0.09	0.19
	a^*	-0.41	0.008	0.000	0.004	0.000	0.000	0.000	0.000	0.01	0.02
	b^*	0.37	0.011	-0.005	0.003	0.000	0.000	0.001	0.001	0.01	0.02
	ΔE		0.014	0.005	0.005	0.066	0.066	0.001	0.001	0.10	0.19

Color Tile	Value		Standard Uncertainty							u_c	U
			u_1	u_2	u_3	u_4	u_5	u_6	u_7		
White	L^*	95.99	0.010	0.000	0.001	0.075	0.075	0.000	0.000	0.11	0.21
	a^*	-0.41	0.007	0.001	0.004	0.000	0.000	0.000	0.001	0.01	0.02
	b^*	1.13	0.010	-0.006	0.004	0.001	0.001	0.001	0.001	0.01	0.02
	ΔE		0.015	0.006	0.006	0.075	0.075	0.001	0.001	0.11	0.21
Deep Pink	L^*	40.47	0.008	0.006	0.001	0.038	0.038	0.005	0.011	0.06	0.11
	a^*	30.12	0.022	-0.008	0.002	0.020	0.020	0.006	0.006	0.04	0.08
	b^*	5.32	0.037	0.004	0.002	0.004	0.004	0.017	0.032	0.05	0.11
	ΔE		0.044	0.011	0.003	0.043	0.043	0.018	0.035	0.09	0.17
Red	L^*	38.00	0.011	0.013	0.001	0.036	0.036	0.011	0.023	0.06	0.12
	a^*	52.65	0.015	-0.019	0.002	0.035	0.035	0.015	0.032	0.06	0.12
	b^*	36.56	0.032	0.018	0.002	0.025	0.025	0.140	0.037	0.15	0.31
	ΔE		0.037	0.029	0.002	0.056	0.056	0.141	0.049	0.18	0.35
Orange	L^*	65.89	0.010	0.002	0.001	0.055	0.055	0.005	0.022	0.08	0.16
	a^*	40.35	0.025	-0.030	0.002	0.027	0.027	0.005	0.036	0.07	0.13
	b^*	60.88	0.086	-0.001	0.002	0.041	0.041	0.085	0.035	0.14	0.28
	ΔE		0.090	0.030	0.004	0.073	0.073	0.086	0.055	0.17	0.35
Yellow	L^*	83.63	0.008	-0.004	0.001	0.066	0.066	0.002	0.010	0.09	0.19
	a^*	-4.49	0.027	0.013	0.004	0.003	0.003	0.006	0.027	0.04	0.08
	b^*	84.87	0.039	-0.050	0.002	0.057	0.057	0.087	0.026	0.14	0.27
	ΔE		0.048	0.052	0.005	0.087	0.087	0.087	0.039	0.17	0.34
Green	L^*	53.44	0.012	-0.002	0.001	0.046	0.046	0.001	0.008	0.07	0.13
	a^*	-35.79	0.044	0.036	0.003	0.024	0.024	0.005	0.012	0.07	0.13
	b^*	15.80	0.036	-0.023	0.002	0.011	0.011	0.010	0.043	0.06	0.13
	ΔE		0.058	0.043	0.004	0.053	0.053	0.011	0.045	0.11	0.23
Diff Green	L^*	53.66	0.013	-0.002	0.001	0.046	0.046	0.001	0.007	0.07	0.13
	a^*	-35.77	0.034	0.037	0.003	0.024	0.024	0.005	0.009	0.06	0.12
	b^*	19.81	0.026	-0.025	0.002	0.013	0.013	0.013	0.042	0.06	0.12
	ΔE		0.044	0.044	0.004	0.054	0.054	0.014	0.044	0.11	0.22
Cyan	L^*	50.88	0.012	0.004	0.001	0.045	0.045	0.002	0.015	0.07	0.13
	a^*	-13.64	0.048	0.000	0.003	0.009	0.009	0.003	0.043	0.07	0.13
	b^*	-33.00	0.030	0.011	0.003	0.022	0.022	0.005	0.032	0.06	0.11
	ΔE		0.058	0.012	0.004	0.051	0.051	0.006	0.055	0.11	0.22
Deep Blue	L^*	9.95	0.005	0.003	0.000	0.017	0.017	0.014	0.004	0.03	0.06
	a^*	22.65	0.119	0.000	0.002	0.015	0.015	0.023	0.025	0.13	0.25
	b^*	-32.64	0.108	-0.005	0.001	0.022	0.022	0.008	0.029	0.12	0.23
	ΔE		0.161	0.006	0.002	0.032	0.032	0.029	0.038	0.17	0.35



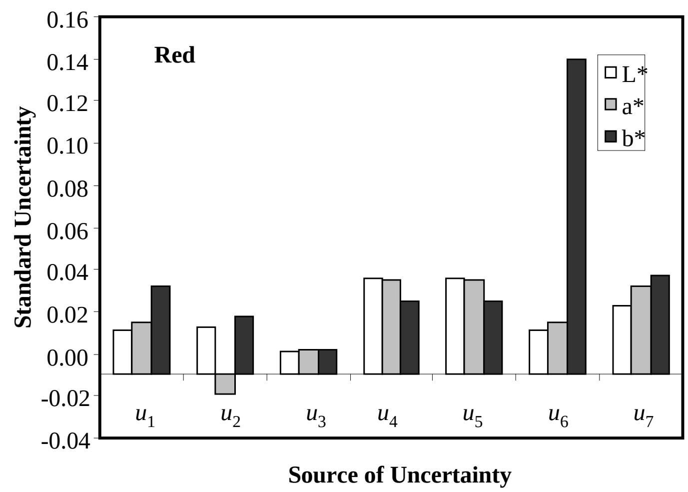


Figure 5.3 Standard uncertainties in L^*, a^*, and b^* caused by the indicated sources of uncertainty for selected samples for CIE Standard Illuminant D65 and the CIE 1964 Standard Observer. The standard uncertainties are u_1 – repeatability, u_2 – bandpass of the monochromator, u_3 – random effects from the calibration of the reference standard, u_4 – systematic effects from the calibration of the reference standard, u_5 – non-linearity of the signals due to non-linearity of the detectors, u_6 – stray light effects, and u_7 – wavelength of the monochromator.

Acknowledgments

The success of the measurement service for 0:45 Color measurements was aided by the efforts of Dr. Gerald Fraser and Dr. Yoshihiro Ohno.

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Appendix A

REPORT OF CALIBRATION

38091S 0:45 Surface Color

for

Color Tile Set

Submitted by:

Any Company, Inc.
Attn.: Ms. Jane Doe
123 Calibration Street
Measurement City, MD 20800-1234

(See your Purchase Order No. 12345, dated January 1, 2006)

1. Description of Calibration Items

One color tile set consisting of fourteen BCRA glossy color tiles manufactured by CERAM Research, 10 cm square, set number NISTCS-XX, supplied by NIST. The set is divided into a wooden box containing twelve colored tiles and a twin box containing a black and a white tile. Each tile in the set is identified by its color designation.

2. Description of Calibration

The surface color of an item depends on the spectral power distribution of the illuminant, the spectral responsivity of the observer, the geometrical conditions of illumination and observation, and the optical properties of the item. Only the last factor depends on the item, and is quantified by the spectral reflectance factor. The spectral reflectance factor R is the ratio of the radiant flux reflected by the item to the radiant flux that would be reflected by a perfect Lambertian diffuser, under identical measurement conditions, as a function of wavelength. The designation 0:45 refers to the bi-directional geometry of the measurement, where the illumination angle is 0º and the viewing angle is 45º.

The calibration items were measured using the NIST 0:45 Reference Reflectometer. A spherical mirror focuses radiant flux from a source through an order-sorting filter onto the entrance slit of a ½ m double-grating monochromator. The beam emerging from the exit slit of the monochromator is incident on a circular aperture and focused by an elliptical mirror in a telecentric arrangement, passes through a Glan-Taylor polarizer, and is incident upon the item. Radiant flux reflected from the item is collected by a receiver consisting of a lens and circular aperture in a telecentric arrangement and a Si photodiode. A sample wheel with twenty positions contains the measured items. At each wavelength and polarization, signals are measured from each position of the sample wheel containing an item. These signals are proportional to the reflected radiant flux. Since the receiver uses a lock-in amplifier to measure the signal from the detector, no dark signals are measured.

Measuring the 0:45 spectral reflectance factor of the calibration items is a relative measurement and therefore requires comparison to a transfer standard with a calibrated 0:45 spectral reflectance factor. The transfer standard is Spectralon, a sintered polytetrafluoroethylene (PTFE) manufactured by Labsphere, Inc., whose 0:45 spectral reflectance factor was determined using the NIST Spectral Tri-function Automated Reference Reflectometer (STARR) [1].

Three Spectralon standards and the calibration items were cleaned with an air bulb and mounted in the sample wheel with the front surfaces aligned normal to the illumination beam and at the same distance from the receiver aperture.

The sampling aperture, defined by the illumination beam, was 10 mm by 12 mm and was located at the center of the reference standards and calibration items. The angle of illumination was 0º from the normal of the item, and the maximum deviation of any ray within the illumination beam from the angle of illumination was 0.92º. The angle of viewing was 45º from the normal of the item, the solid angle of collection was 0.00176 sr, and the maximum deviation of any ray within the receiver beam from the angle of viewing was 1.36º. This geometry is designated as 0:45.

The reference standards and calibration items were measured at wavelengths from 380 nm to 780 nm every 5 nm. The spectral bandwidth of the illumination beam was 5 nm. The source was a Xe arc lamp for wavelengths of 460 nm and shorter and a quartz-tungsten-halogen incandescent lamp for longer wavelengths. Each reference standard and calibration item was measured three times for polarizations of the illumination beam both parallel and perpendicular to the plane of illumination

3. Results of Calibration

The reflectance factor R at each wavelength λ and polarization σ is given by

$$R(\lambda,\sigma) = \frac{S(\lambda,\sigma)}{S_s(\lambda,\sigma)} \cdot R_s(\lambda,\sigma) \quad , \qquad 3.1$$

where S and S_s are the measured signals from the item and reference standard, respectively, and R_s is the reflectance factor of the reference standard.

The final 0:45 spectral reflectance factor was obtained by averaging the values from multiple scans. The certified 0:45 spectral reflectance factor of each calibration item, measured according to the details given above, is given in Tables 1 to 14.

The tristimulus values *X*, *Y*, and *Z* of each item were calculated for CIE standard illuminant D65 and CIE 1931 standard observer [2]. The chromaticity coordinates *x* and *y* were derived from the tristimulus values [3].

The tristimulus values, for reflectance factors regularly spaced in wavelength, are given by

$$X = \sum_{i=1}^{m} W_{\mathrm{x},i} \cdot R_i \quad , \tag{3.2}$$

$$Y = \sum_{i=1}^{m} W_{\mathrm{y},i} \cdot R_i \quad , \text{ and} \tag{3.3}$$

$$Z = \sum_{i=1}^{m} W_{\mathrm{z},i} \cdot R_i \quad , \tag{3.4}$$

where *i* indexes the wavelengths, $W_{\mathrm{x},i}$, $W_{\mathrm{y},i}$, and $W_{\mathrm{z},i}$ are the normalized tristimulus weighting factors for a particular illuminant and observer combination, and R_i is the spectral reflectance factor. The chromaticity coordinates are given by

$$x = \frac{X}{X + Y + Z} \quad \text{and} \tag{3.5}$$

$$y = \frac{Y}{X + Y + Z} \, . \tag{3.6}$$

The tristimulus value *Y* and chromaticity coordinates *x* and *y* for CIE standard illuminant D65 and CIE 1931 standard observer of each of the calibrated items is given in Table 15.

Uncertainties were calculated according to the procedures outlined in Reference 4 and 5]. From the measurement equation for the spectral reflectance factor, Eq. (3.1), uncertainties in *S*, S_s, R_s, and λ all contribute to an uncertainty in *R*. An important consideration for determining the uncertainty in *R* is correlations between signals *S* and S_s at the same wavelength. The uncertainties in *Y*, *x*, and *y* were calculated by propagating the uncertainties in the spectral reflectance factor thorough the calculations, including correlations between the uncertainties in *R* at different wavelengths.

The sources of uncertainty are signal noise, offset in the signal, and uncertainties in the reference standard and the wavelength. Signal noise is the result of random processes in both the source and the detector. Offsets in the signal include non-linearity and stray light. Non-linearity is a deviation of the signal from proportionality with the radiant flux as the signal changes value. Stray light is radiant flux that reaches the detector at wavelengths outside the nominal spectral bandwidth of the instrument. The reference standard has an uncertainty from its calibration, and there is an uncertainty associated with the wavelength setting of the measuring instrument.

The uncertainties from signal noise include source stability and detector noise. The uncertainty contributions caused by these effects were evaluated by multiple measurements of the items. The uncertainties from non-linearity, stray light, wavelength, and reference standard were evaluated as part of the characterization of the 0:45 Reference Reflectometer and their values are given in Table 16.

The expanded uncertainty was obtained from the root-sum-square of the uncertainty contributions multiplied by a coverage factor k = 2. The expanded uncertainty in 0:45 spectral reflectance factor of each calibration item is given in Tables 1 to 14. The expanded uncertainties in tristimulus value and chromaticity coordinates of each calibration item are given in Table 15.

4. General Information

1) The values in Tables 1 to 15 apply only to the central 10 mm by 12 mm area of the calibration item.
2) This calibration report may not be reproduced except in full without the written consent of this Laboratory.

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Table 1. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (*k* = 2) as a function of wavelength λ of the Black color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0051	0.0007	515	0.0067	0.0003	650	0.0058	0.0001
385	0.0055	0.0012	520	0.0067	0.0001	655	0.0059	0.0001
390	0.0056	0.0011	525	0.0067	0.0001	660	0.0060	0.0001
395	0.0056	0.0008	530	0.0068	0.0000	665	0.0062	0.0001
400	0.0059	0.0008	535	0.0070	0.0001	670	0.0066	0.0001
405	0.0059	0.0007	540	0.0069	0.0001	675	0.0070	0.0001
410	0.0062	0.0003	545	0.0070	0.0002	680	0.0078	0.0001
415	0.0061	0.0002	550	0.0068	0.0002	685	0.0088	0.0001
420	0.0060	0.0003	555	0.0067	0.0001	690	0.0100	0.0001
425	0.0061	0.0004	560	0.0065	0.0001	695	0.0115	0.0001
430	0.0061	0.0002	565	0.0062	0.0001	700	0.0133	0.0001
435	0.0061	0.0000	570	0.0060	0.0001	705	0.0151	0.0001
440	0.0062	0.0001	575	0.0058	0.0002	710	0.0171	0.0001
445	0.0062	0.0001	580	0.0056	0.0002	715	0.0190	0.0002
450	0.0062	0.0001	585	0.0056	0.0001	720	0.0209	0.0002
455	0.0063	0.0001	590	0.0055	0.0001	725	0.0229	0.0002
460	0.0062	0.0004	595	0.0054	0.0000	730	0.0247	0.0002
465	0.0063	0.0005	600	0.0053	0.0001	735	0.0265	0.0002
470	0.0062	0.0002	605	0.0052	0.0001	740	0.0282	0.0003
475	0.0064	0.0007	610	0.0051	0.0001	745	0.0298	0.0002
480	0.0062	0.0004	615	0.0052	0.0001	750	0.0313	0.0002
485	0.0061	0.0002	620	0.0053	0.0001	755	0.0329	0.0002
490	0.0062	0.0004	625	0.0055	0.0001	760	0.0344	0.0002
495	0.0062	0.0005	630	0.0057	0.0001	765	0.0359	0.0002
500	0.0063	0.0004	635	0.0057	0.0001	770	0.0373	0.0002
505	0.0063	0.0002	640	0.0058	0.0001	775	0.0388	0.0003
510	0.0065	0.0001	645	0.0059	0.0001	780	0.0404	0.0003

Table 2. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Cyan color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.1665	0.0020	515	0.3246	0.0019	650	0.0712	0.0004
385	0.1911	0.0017	520	0.3007	0.0019	655	0.0722	0.0004
390	0.2164	0.0018	525	0.2769	0.0017	660	0.0735	0.0004
395	0.2404	0.0030	530	0.2540	0.0017	665	0.0753	0.0004
400	0.2627	0.0024	535	0.2322	0.0014	670	0.0776	0.0005
405	0.2846	0.0020	540	0.2121	0.0013	675	0.0804	0.0005
410	0.3050	0.0021	545	0.1935	0.0012	680	0.0838	0.0005
415	0.3235	0.0023	550	0.1767	0.0011	685	0.0877	0.0005
420	0.3413	0.0021	555	0.1618	0.0010	690	0.0922	0.0006
425	0.3570	0.0027	560	0.1483	0.0009	695	0.0974	0.0006
430	0.3719	0.0022	565	0.1365	0.0008	700	0.1032	0.0006
435	0.3857	0.0023	570	0.1260	0.0008	705	0.1095	0.0006
440	0.3984	0.0026	575	0.1168	0.0007	710	0.1159	0.0007
445	0.4095	0.0024	580	0.1088	0.0007	715	0.1218	0.0007
450	0.4200	0.0025	585	0.1018	0.0006	720	0.1269	0.0007
455	0.4287	0.0025	590	0.0958	0.0006	725	0.1311	0.0007
460	0.4370	0.0026	595	0.0906	0.0005	730	0.1342	0.0008
465	0.4416	0.0027	600	0.0862	0.0005	735	0.1364	0.0008
470	0.4432	0.0026	605	0.0824	0.0005	740	0.1376	0.0008
475	0.4428	0.0026	610	0.0792	0.0005	745	0.1381	0.0008
480	0.4387	0.0028	615	0.0766	0.0005	750	0.1380	0.0008
485	0.4316	0.0025	620	0.0746	0.0004	755	0.1374	0.0008
490	0.4208	0.0026	625	0.0729	0.0004	760	0.1365	0.0008
495	0.4069	0.0024	630	0.0717	0.0004	765	0.1352	0.0008
500	0.3900	0.0023	635	0.0710	0.0004	770	0.1340	0.0008
505	0.3700	0.0022	640	0.0707	0.0004	775	0.1326	0.0008
510	0.3480	0.0022	645	0.0708	0.0004	780	0.1314	0.0008

Table 3. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Deep Blue color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.1169	0.0038	515	0.0116	0.0003	650	0.0078	0.0002
385	0.1253	0.0023	520	0.0114	0.0001	655	0.0080	0.0001
390	0.1322	0.0013	525	0.0113	0.0003	660	0.0085	0.0001
395	0.1379	0.0016	530	0.0114	0.0001	665	0.0092	0.0001
400	0.1407	0.0010	535	0.0116	0.0002	670	0.0101	0.0001
405	0.1410	0.0012	540	0.0120	0.0001	675	0.0117	0.0001
410	0.1388	0.0010	545	0.0121	0.0001	680	0.0142	0.0001
415	0.1336	0.0015	550	0.0121	0.0001	685	0.0182	0.0002
420	0.1256	0.0010	555	0.0115	0.0001	690	0.0246	0.0003
425	0.1160	0.0012	560	0.0106	0.0002	695	0.0342	0.0030
430	0.1050	0.0011	565	0.0096	0.0001	700	0.0508	0.0005
435	0.0933	0.0010	570	0.0088	0.0001	705	0.0737	0.0007
440	0.0816	0.0009	575	0.0080	0.0001	710	0.1049	0.0010
445	0.0703	0.0009	580	0.0075	0.0001	715	0.1444	0.0012
450	0.0593	0.0008	585	0.0072	0.0001	720	0.1913	0.0015
455	0.0500	0.0007	590	0.0070	0.0001	725	0.2436	0.0019
460	0.0399	0.0008	595	0.0070	0.0001	730	0.2981	0.0021
465	0.0329	0.0008	600	0.0072	0.0000	735	0.3519	0.0024
470	0.0273	0.0007	605	0.0073	0.0001	740	0.4012	0.0026
475	0.0232	0.0004	610	0.0074	0.0001	745	0.4440	0.0027
480	0.0197	0.0018	615	0.0075	0.0001	750	0.4785	0.0028
485	0.0178	0.0003	620	0.0075	0.0001	755	0.5042	0.0029
490	0.0162	0.0003	625	0.0076	0.0001	760	0.5221	0.0030
495	0.0148	0.0005	630	0.0075	0.0000	765	0.5331	0.0034
500	0.0137	0.0003	635	0.0075	0.0000	770	0.5379	0.0031
505	0.0124	0.0011	640	0.0076	0.0002	775	0.5392	0.0031
510	0.0121	0.0002	645	0.0074	0.0007	780	0.5368	0.0031

Table 4. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Deep Gray color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0452	0.0028	515	0.0491	0.0003	650	0.0540	0.0003
385	0.0459	0.0019	520	0.0496	0.0003	655	0.0543	0.0003
390	0.0466	0.0011	525	0.0501	0.0003	660	0.0551	0.0003
395	0.0470	0.0011	530	0.0507	0.0003	665	0.0564	0.0003
400	0.0477	0.0008	535	0.0513	0.0004	670	0.0585	0.0003
405	0.0477	0.0006	540	0.0520	0.0003	675	0.0615	0.0004
410	0.0479	0.0004	545	0.0525	0.0003	680	0.0654	0.0004
415	0.0480	0.0006	550	0.0527	0.0003	685	0.0702	0.0004
420	0.0479	0.0005	555	0.0526	0.0003	690	0.0758	0.0005
425	0.0479	0.0003	560	0.0522	0.0003	695	0.0819	0.0005
430	0.0478	0.0004	565	0.0516	0.0003	700	0.0884	0.0005
435	0.0478	0.0004	570	0.0510	0.0003	705	0.0954	0.0006
440	0.0479	0.0003	575	0.0507	0.0003	710	0.1028	0.0006
445	0.0479	0.0003	580	0.0505	0.0003	715	0.1104	0.0007
450	0.0479	0.0003	585	0.0503	0.0003	720	0.1182	0.0007
455	0.0482	0.0003	590	0.0503	0.0003	725	0.1262	0.0007
460	0.0482	0.0008	595	0.0501	0.0003	730	0.1343	0.0008
465	0.0485	0.0010	600	0.0498	0.0003	735	0.1426	0.0009
470	0.0483	0.0009	605	0.0495	0.0003	740	0.1507	0.0009
475	0.0484	0.0006	610	0.0495	0.0003	745	0.1585	0.0009
480	0.0484	0.0006	615	0.0499	0.0003	750	0.1657	0.0010
485	0.0484	0.0003	620	0.0507	0.0003	755	0.1721	0.0010
490	0.0484	0.0004	625	0.0515	0.0003	760	0.1779	0.0010
495	0.0483	0.0004	630	0.0523	0.0003	765	0.1827	0.0011
500	0.0484	0.0003	635	0.0529	0.0003	770	0.1870	0.0011
505	0.0487	0.0004	640	0.0534	0.0003	775	0.1909	0.0011
510	0.0488	0.0004	645	0.0537	0.0003	780	0.1946	0.0012

Table 5. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Deep Pink color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.1483	0.0034	515	0.0648	0.0005	650	0.3584	0.0021
385	0.1487	0.0018	520	0.0650	0.0004	655	0.3765	0.0022
390	0.1489	0.0017	525	0.0658	0.0004	660	0.3944	0.0023
395	0.1471	0.0013	530	0.0672	0.0005	665	0.4114	0.0024
400	0.1459	0.0012	535	0.0694	0.0005	670	0.4276	0.0026
405	0.1435	0.0011	540	0.0723	0.0004	675	0.4428	0.0026
410	0.1400	0.0015	545	0.0758	0.0004	680	0.4567	0.0026
415	0.1358	0.0011	550	0.0800	0.0005	685	0.4690	0.0028
420	0.1311	0.0013	555	0.0849	0.0005	690	0.4797	0.0028
425	0.1260	0.0011	560	0.0905	0.0005	695	0.4899	0.0028
430	0.1207	0.0008	565	0.0970	0.0006	700	0.4990	0.0028
435	0.1154	0.0009	570	0.1046	0.0008	705	0.5064	0.0033
440	0.1102	0.0008	575	0.1129	0.0007	710	0.5138	0.0031
445	0.1052	0.0006	580	0.1226	0.0007	715	0.5191	0.0036
450	0.1002	0.0007	585	0.1335	0.0008	720	0.5236	0.0030
455	0.0957	0.0008	590	0.1458	0.0009	725	0.5271	0.0030
460	0.0901	0.0008	595	0.1593	0.0010	730	0.5290	0.0031
465	0.0861	0.0007	600	0.1742	0.0012	735	0.5308	0.0032
470	0.0824	0.0007	605	0.1902	0.0012	740	0.5310	0.0030
475	0.0789	0.0008	610	0.2073	0.0013	745	0.5305	0.0031
480	0.0759	0.0008	615	0.2252	0.0014	750	0.5296	0.0031
485	0.0732	0.0006	620	0.2438	0.0015	755	0.5282	0.0030
490	0.0696	0.0063	625	0.2630	0.0015	760	0.5264	0.0030
495	0.0688	0.0004	630	0.2822	0.0017	765	0.5241	0.0031
500	0.0672	0.0005	635	0.3016	0.0018	770	0.5217	0.0030
505	0.0646	0.0055	640	0.3209	0.0019	775	0.5187	0.0030
510	0.0651	0.0005	645	0.3399	0.0020	780	0.5158	0.0029

Table 6. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Diff Gray color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.2002	0.0026	515	0.2663	0.0014	650	0.2538	0.0015
385	0.2063	0.0024	520	0.2668	0.0015	655	0.2534	0.0015
390	0.2100	0.0013	525	0.2670	0.0015	660	0.2538	0.0015
395	0.2137	0.0014	530	0.2672	0.0015	665	0.2542	0.0015
400	0.2173	0.0018	535	0.2671	0.0015	670	0.2549	0.0014
405	0.2203	0.0016	540	0.2672	0.0015	675	0.2557	0.0015
410	0.2236	0.0014	545	0.2668	0.0015	680	0.2567	0.0015
415	0.2264	0.0015	550	0.2661	0.0015	685	0.2577	0.0015
420	0.2292	0.0014	555	0.2651	0.0015	690	0.2586	0.0015
425	0.2322	0.0015	560	0.2637	0.0015	695	0.2596	0.0015
430	0.2348	0.0015	565	0.2622	0.0015	700	0.2605	0.0015
435	0.2377	0.0015	570	0.2606	0.0015	705	0.2610	0.0015
440	0.2405	0.0015	575	0.2590	0.0015	710	0.2612	0.0015
445	0.2433	0.0014	580	0.2577	0.0014	715	0.2612	0.0015
450	0.2459	0.0015	585	0.2566	0.0015	720	0.2611	0.0015
455	0.2483	0.0015	590	0.2562	0.0015	725	0.2607	0.0015
460	0.2508	0.0015	595	0.2561	0.0015	730	0.2602	0.0015
465	0.2530	0.0015	600	0.2561	0.0016	735	0.2595	0.0014
470	0.2547	0.0015	605	0.2561	0.0015	740	0.2585	0.0015
475	0.2567	0.0015	610	0.2562	0.0015	745	0.2579	0.0015
480	0.2588	0.0015	615	0.2561	0.0015	750	0.2569	0.0014
485	0.2603	0.0014	620	0.2560	0.0015	755	0.2557	0.0014
490	0.2620	0.0015	625	0.2557	0.0015	760	0.2546	0.0014
495	0.2634	0.0015	630	0.2554	0.0015	765	0.2534	0.0015
500	0.2645	0.0015	635	0.2548	0.0015	770	0.2521	0.0014
505	0.2655	0.0015	640	0.2544	0.0015	775	0.2509	0.0014
510	0.2661	0.0015	645	0.2543	0.0015	780	0.2496	0.0014

Table 7. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (*k* = 2) as a function of wavelength λ of the Diff Green color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0511	0.0027	515	0.3366	0.0020	650	0.1127	0.0006
385	0.0544	0.0020	520	0.3328	0.0020	655	0.1139	0.0006
390	0.0565	0.0020	525	0.3225	0.0019	660	0.1157	0.0007
395	0.0584	0.0009	530	0.3079	0.0018	665	0.1182	0.0006
400	0.0604	0.0009	535	0.2908	0.0018	670	0.1212	0.0007
405	0.0624	0.0008	540	0.2731	0.0016	675	0.1249	0.0007
410	0.0641	0.0008	545	0.2549	0.0015	680	0.1293	0.0007
415	0.0661	0.0007	550	0.2377	0.0014	685	0.1345	0.0008
420	0.0685	0.0006	555	0.2215	0.0013	690	0.1402	0.0008
425	0.0712	0.0006	560	0.2066	0.0012	695	0.1468	0.0008
430	0.0746	0.0006	565	0.1931	0.0011	700	0.1542	0.0009
435	0.0787	0.0006	570	0.1808	0.0010	705	0.1620	0.0009
440	0.0835	0.0007	575	0.1696	0.0011	710	0.1697	0.0010
445	0.0893	0.0007	580	0.1599	0.0009	715	0.1769	0.0010
450	0.0966	0.0008	585	0.1513	0.0009	720	0.1830	0.0010
455	0.1051	0.0010	590	0.1438	0.0008	725	0.1880	0.0011
460	0.1182	0.0009	595	0.1373	0.0008	730	0.1914	0.0011
465	0.1315	0.0012	600	0.1318	0.0008	735	0.1939	0.0011
470	0.1479	0.0012	605	0.1269	0.0007	740	0.1953	0.0011
475	0.1675	0.0012	610	0.1229	0.0007	745	0.1958	0.0011
480	0.1901	0.0015	615	0.1195	0.0007	750	0.1956	0.0011
485	0.2159	0.0015	620	0.1168	0.0007	755	0.1949	0.0011
490	0.2440	0.0016	625	0.1147	0.0006	760	0.1938	0.0011
495	0.2730	0.0018	630	0.1133	0.0006	765	0.1923	0.0011
500	0.2991	0.0020	635	0.1123	0.0006	770	0.1907	0.0011
505	0.3199	0.0019	640	0.1119	0.0006	775	0.1891	0.0010
510	0.3326	0.0020	645	0.1121	0.0006	780	0.1875	0.0011

Table 8. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Green color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0584	0.0041	515	0.3401	0.0020	650	0.1075	0.0006
385	0.0616	0.0018	520	0.3335	0.0020	655	0.1086	0.0007
390	0.0653	0.0017	525	0.3212	0.0020	660	0.1104	0.0006
395	0.0675	0.0012	530	0.3052	0.0019	665	0.1129	0.0007
400	0.0698	0.0010	535	0.2871	0.0018	670	0.1160	0.0007
405	0.0721	0.0007	540	0.2686	0.0017	675	0.1196	0.0007
410	0.0744	0.0006	545	0.2502	0.0015	680	0.1240	0.0007
415	0.0768	0.0007	550	0.2326	0.0014	685	0.1291	0.0008
420	0.0796	0.0006	555	0.2163	0.0013	690	0.1350	0.0008
425	0.0828	0.0006	560	0.2012	0.0012	695	0.1416	0.0008
430	0.0863	0.0007	565	0.1875	0.0011	700	0.1489	0.0009
435	0.0909	0.0007	570	0.1752	0.0010	705	0.1567	0.0009
440	0.0962	0.0007	575	0.1641	0.0010	710	0.1645	0.0010
445	0.1026	0.0008	580	0.1543	0.0009	715	0.1717	0.0010
450	0.1106	0.0010	585	0.1457	0.0009	720	0.1779	0.0010
455	0.1197	0.0010	590	0.1383	0.0008	725	0.1828	0.0011
460	0.1339	0.0010	595	0.1318	0.0008	730	0.1865	0.0011
465	0.1481	0.0012	600	0.1264	0.0008	735	0.1889	0.0011
470	0.1653	0.0012	605	0.1215	0.0007	740	0.1903	0.0011
475	0.1857	0.0013	610	0.1175	0.0007	745	0.1908	0.0011
480	0.2088	0.0014	615	0.1142	0.0007	750	0.1907	0.0011
485	0.2347	0.0015	620	0.1115	0.0006	755	0.1899	0.0011
490	0.2624	0.0017	625	0.1095	0.0006	760	0.1888	0.0011
495	0.2897	0.0018	630	0.1080	0.0006	765	0.1873	0.0011
500	0.3130	0.0020	635	0.1071	0.0006	770	0.1857	0.0011
505	0.3302	0.0020	640	0.1067	0.0006	775	0.1841	0.0010
510	0.3397	0.0020	645	0.1068	0.0006	780	0.1826	0.0011

Table 9. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Mid Gray color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.2162	0.0023	515	0.2533	0.0015	650	0.2548	0.0015
385	0.2217	0.0026	520	0.2540	0.0015	655	0.2544	0.0015
390	0.2255	0.0015	525	0.2547	0.0015	660	0.2543	0.0015
395	0.2298	0.0016	530	0.2555	0.0015	665	0.2545	0.0015
400	0.2337	0.0014	535	0.2563	0.0015	670	0.2547	0.0015
405	0.2368	0.0014	540	0.2572	0.0016	675	0.2552	0.0015
410	0.2399	0.0017	545	0.2579	0.0015	680	0.2556	0.0015
415	0.2424	0.0014	550	0.2581	0.0015	685	0.2562	0.0015
420	0.2451	0.0015	555	0.2582	0.0015	690	0.2566	0.0015
425	0.2476	0.0015	560	0.2577	0.0015	695	0.2569	0.0015
430	0.2496	0.0016	565	0.2573	0.0015	700	0.2570	0.0015
435	0.2514	0.0016	570	0.2565	0.0015	705	0.2568	0.0015
440	0.2525	0.0015	575	0.2556	0.0015	710	0.2565	0.0015
445	0.2539	0.0015	580	0.2551	0.0015	715	0.2558	0.0015
450	0.2544	0.0016	585	0.2548	0.0015	720	0.2551	0.0015
455	0.2548	0.0015	590	0.2548	0.0014	725	0.2542	0.0014
460	0.2547	0.0015	595	0.2552	0.0015	730	0.2534	0.0014
465	0.2544	0.0018	600	0.2558	0.0015	735	0.2523	0.0014
470	0.2536	0.0016	605	0.2563	0.0015	740	0.2514	0.0014
475	0.2532	0.0015	610	0.2566	0.0015	745	0.2503	0.0014
480	0.2528	0.0016	615	0.2568	0.0015	750	0.2493	0.0014
485	0.2525	0.0015	620	0.2570	0.0015	755	0.2481	0.0014
490	0.2524	0.0014	625	0.2569	0.0015	760	0.2471	0.0014
495	0.2524	0.0015	630	0.2567	0.0015	765	0.2458	0.0014
500	0.2525	0.0015	635	0.2562	0.0015	770	0.2445	0.0014
505	0.2526	0.0015	640	0.2558	0.0015	775	0.2431	0.0014
510	0.2530	0.0015	645	0.2555	0.0015	780	0.2418	0.0014

Table 10. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Orange color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0520	0.0066	515	0.0806	0.0006	650	0.7699	0.0044
385	0.0529	0.0042	520	0.0838	0.0005	655	0.7742	0.0044
390	0.0545	0.0028	525	0.0876	0.0006	660	0.7789	0.0045
395	0.0555	0.0021	530	0.0937	0.0006	665	0.7834	0.0045
400	0.0566	0.0014	535	0.1051	0.0007	670	0.7871	0.0045
405	0.0573	0.0013	540	0.1260	0.0010	675	0.7913	0.0046
410	0.0581	0.0011	545	0.1608	0.0014	680	0.7947	0.0045
415	0.0591	0.0011	550	0.2124	0.0018	685	0.7983	0.0047
420	0.0601	0.0010	555	0.2791	0.0023	690	0.8015	0.0046
425	0.0607	0.0007	560	0.3539	0.0026	695	0.8047	0.0046
430	0.0616	0.0009	565	0.4280	0.0029	700	0.8081	0.0046
435	0.0625	0.0008	570	0.4934	0.0031	705	0.8113	0.0046
440	0.0623	0.0059	575	0.5475	0.0034	710	0.8150	0.0047
445	0.0643	0.0008	580	0.5903	0.0035	715	0.8180	0.0047
450	0.0656	0.0009	585	0.6240	0.0036	720	0.8211	0.0047
455	0.0666	0.0009	590	0.6512	0.0038	725	0.8231	0.0047
460	0.0617	0.0010	595	0.6726	0.0039	730	0.8244	0.0047
465	0.0625	0.0010	600	0.6902	0.0040	735	0.8255	0.0048
470	0.0634	0.0008	605	0.7041	0.0040	740	0.8263	0.0047
475	0.0641	0.0009	610	0.7155	0.0041	745	0.8273	0.0047
480	0.0649	0.0006	615	0.7257	0.0042	750	0.8281	0.0048
485	0.0657	0.0006	620	0.7336	0.0046	755	0.8293	0.0047
490	0.0670	0.0005	625	0.7415	0.0042	760	0.8305	0.0047
495	0.0681	0.0006	630	0.7486	0.0043	765	0.8308	0.0047
500	0.0700	0.0006	635	0.7543	0.0043	770	0.8318	0.0048
505	0.0731	0.0006	640	0.7601	0.0043	775	0.8323	0.0047
510	0.0769	0.0006	645	0.7651	0.0044	780	0.8329	0.0048

Table 11. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Pale Gray color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.5670	0.0044	515	0.6306	0.0036	650	0.6273	0.0036
385	0.5783	0.0039	520	0.6310	0.0036	655	0.6269	0.0036
390	0.5864	0.0047	525	0.6312	0.0036	660	0.6270	0.0036
395	0.5935	0.0042	530	0.6318	0.0036	665	0.6271	0.0036
400	0.5994	0.0034	535	0.6322	0.0036	670	0.6271	0.0036
405	0.6043	0.0035	540	0.6324	0.0037	675	0.6278	0.0036
410	0.6081	0.0041	545	0.6325	0.0037	680	0.6283	0.0036
415	0.6113	0.0043	550	0.6320	0.0036	685	0.6286	0.0036
420	0.6148	0.0039	555	0.6316	0.0036	690	0.6291	0.0037
425	0.6175	0.0037	560	0.6307	0.0036	695	0.6289	0.0038
430	0.6203	0.0040	565	0.6297	0.0036	700	0.6292	0.0036
435	0.6229	0.0040	570	0.6287	0.0036	705	0.6286	0.0036
440	0.6236	0.0036	575	0.6276	0.0036	710	0.6284	0.0036
445	0.6261	0.0037	580	0.6272	0.0037	715	0.6278	0.0036
450	0.6269	0.0041	585	0.6266	0.0037	720	0.6273	0.0036
455	0.6282	0.0039	590	0.6270	0.0036	725	0.6263	0.0036
460	0.6285	0.0036	595	0.6272	0.0036	730	0.6252	0.0036
465	0.6286	0.0036	600	0.6280	0.0038	735	0.6242	0.0036
470	0.6288	0.0036	605	0.6280	0.0036	740	0.6234	0.0036
475	0.6288	0.0036	610	0.6285	0.0036	745	0.6224	0.0036
480	0.6286	0.0036	615	0.6287	0.0036	750	0.6212	0.0036
485	0.6288	0.0037	620	0.6290	0.0036	755	0.6201	0.0035
490	0.6289	0.0036	625	0.6289	0.0036	760	0.6187	0.0038
495	0.6292	0.0036	630	0.6286	0.0036	765	0.6176	0.0035
500	0.6292	0.0039	635	0.6282	0.0036	770	0.6164	0.0036
505	0.6300	0.0036	640	0.6280	0.0036	775	0.6150	0.0035
510	0.6302	0.0036	645	0.6277	0.0036	780	0.6139	0.0035

Table 12. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Red color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0156	0.0058	515	0.0269	0.0004	650	0.6471	0.0037
385	0.0165	0.0036	520	0.0280	0.0003	655	0.6619	0.0038
390	0.0170	0.0024	525	0.0294	0.0003	660	0.6764	0.0039
395	0.0181	0.0018	530	0.0309	0.0003	665	0.6891	0.0039
400	0.0187	0.0014	535	0.0324	0.0003	670	0.7009	0.0040
405	0.0191	0.0012	540	0.0337	0.0003	675	0.7111	0.0041
410	0.0196	0.0010	545	0.0350	0.0003	680	0.7207	0.0041
415	0.0202	0.0007	550	0.0364	0.0003	685	0.7297	0.0043
420	0.0206	0.0007	555	0.0373	0.0035	690	0.7373	0.0042
425	0.0208	0.0005	560	0.0405	0.0003	695	0.7460	0.0043
430	0.0212	0.0005	565	0.0442	0.0003	700	0.7544	0.0044
435	0.0214	0.0004	570	0.0500	0.0003	705	0.7623	0.0044
440	0.0218	0.0004	575	0.0584	0.0004	710	0.7703	0.0044
445	0.0217	0.0020	580	0.0699	0.0005	715	0.7782	0.0045
450	0.0224	0.0003	585	0.0851	0.0006	720	0.7845	0.0045
455	0.0228	0.0003	590	0.1049	0.0008	725	0.7891	0.0045
460	0.0223	0.0010	595	0.1314	0.0010	730	0.7914	0.0045
465	0.0228	0.0009	600	0.1674	0.0014	735	0.7925	0.0047
470	0.0231	0.0006	605	0.2159	0.0019	740	0.7932	0.0048
475	0.0233	0.0005	610	0.2773	0.0022	745	0.7944	0.0045
480	0.0236	0.0005	615	0.3480	0.0026	750	0.7957	0.0046
485	0.0235	0.0022	620	0.4193	0.0029	755	0.7967	0.0048
490	0.0248	0.0004	625	0.4834	0.0031	760	0.7978	0.0045
495	0.0251	0.0003	630	0.5355	0.0032	765	0.7986	0.0046
500	0.0252	0.0004	635	0.5753	0.0033	770	0.7991	0.0046
505	0.0255	0.0004	640	0.6057	0.0035	775	0.7996	0.0046
510	0.0262	0.0003	645	0.6292	0.0037	780	0.8002	0.0046

Table 13. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (*k* = 2) as a function of wavelength *λ* of the White color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	*λ* [nm]	*R*	*U*	*λ* [nm]	*R*	*U*
380	0.7564	0.0050	515	0.8988	0.0051	650	0.9028	0.0051
385	0.7791	0.0053	520	0.8992	0.0052	655	0.9028	0.0051
390	0.8014	0.0053	525	0.8998	0.0052	660	0.9035	0.0052
395	0.8199	0.0048	530	0.9003	0.0051	665	0.9047	0.0052
400	0.8356	0.0050	535	0.9008	0.0052	670	0.9052	0.0052
405	0.8482	0.0055	540	0.9008	0.0052	675	0.9057	0.0052
410	0.8577	0.0053	545	0.9009	0.0052	680	0.9064	0.0052
415	0.8631	0.0050	550	0.9010	0.0052	685	0.9067	0.0052
420	0.8687	0.0060	555	0.9010	0.0053	690	0.9069	0.0052
425	0.8736	0.0052	560	0.9010	0.0052	695	0.9069	0.0053
430	0.8764	0.0051	565	0.9010	0.0051	700	0.9075	0.0052
435	0.8775	0.0052	570	0.9002	0.0051	705	0.9076	0.0052
440	0.8798	0.0052	575	0.8996	0.0051	710	0.9076	0.0054
445	0.8811	0.0052	580	0.8994	0.0051	715	0.9084	0.0052
450	0.8824	0.0054	585	0.8994	0.0052	720	0.9082	0.0052
455	0.8860	0.0058	590	0.9006	0.0052	725	0.9084	0.0052
460	0.8869	0.0051	595	0.9010	0.0051	730	0.9084	0.0052
465	0.8896	0.0051	600	0.9021	0.0054	735	0.9085	0.0052
470	0.8910	0.0052	605	0.9017	0.0052	740	0.9082	0.0052
475	0.8924	0.0051	610	0.9019	0.0052	745	0.9081	0.0052
480	0.8935	0.0051	615	0.9020	0.0052	750	0.9084	0.0052
485	0.8942	0.0053	620	0.9020	0.0052	755	0.9084	0.0052
490	0.8952	0.0051	625	0.9026	0.0051	760	0.9084	0.0052
495	0.8962	0.0052	630	0.9022	0.0052	765	0.9079	0.0052
500	0.8971	0.0052	635	0.9021	0.0052	770	0.9082	0.0052
505	0.8980	0.0051	640	0.9026	0.0052	775	0.9079	0.0052
510	0.8986	0.0051	645	0.9032	0.0051	780	0.9078	0.0052

Table 14. 0:45 spectral reflectance factor *R* and expanded uncertainty *U* (k = 2) as a function of wavelength λ of the Yellow color tile, set number NISTCS-XX

λ [nm]	*R*	*U*	λ [nm]	*R*	*U*	λ [nm]	*R*	*U*
380	0.0240	0.0075	515	0.4630	0.0030	650	0.7904	0.0045
385	0.0249	0.0051	520	0.5179	0.0033	655	0.7916	0.0047
390	0.0253	0.0034	525	0.5656	0.0034	660	0.7943	0.0046
395	0.0252	0.0023	530	0.6050	0.0036	665	0.7966	0.0046
400	0.0255	0.0017	535	0.6364	0.0037	670	0.7989	0.0047
405	0.0262	0.0015	540	0.6611	0.0040	675	0.8011	0.0046
410	0.0270	0.0013	545	0.6802	0.0040	680	0.8028	0.0046
415	0.0277	0.0010	550	0.6951	0.0040	685	0.8047	0.0046
420	0.0289	0.0009	555	0.7072	0.0041	690	0.8060	0.0047
425	0.0304	0.0008	560	0.7165	0.0041	695	0.8077	0.0046
430	0.0322	0.0007	565	0.7249	0.0042	700	0.8095	0.0046
435	0.0345	0.0006	570	0.7309	0.0042	705	0.8107	0.0046
440	0.0375	0.0005	575	0.7326	0.0042	710	0.8125	0.0046
445	0.0413	0.0006	580	0.7361	0.0042	715	0.8137	0.0047
450	0.0463	0.0005	585	0.7404	0.0042	720	0.8149	0.0046
455	0.0522	0.0007	590	0.7455	0.0043	725	0.8159	0.0047
460	0.0619	0.0010	595	0.7520	0.0043	730	0.8168	0.0047
465	0.0728	0.0011	600	0.7591	0.0045	735	0.8163	0.0048
470	0.0863	0.0009	605	0.7644	0.0044	740	0.8144	0.0047
475	0.1040	0.0009	610	0.7694	0.0045	745	0.8167	0.0047
480	0.1265	0.0011	615	0.7735	0.0044	750	0.8158	0.0047
485	0.1550	0.0012	620	0.7771	0.0044	755	0.8184	0.0047
490	0.1911	0.0015	625	0.7796	0.0047	760	0.8204	0.0047
495	0.2348	0.0017	630	0.7824	0.0045	765	0.8228	0.0048
500	0.2857	0.0022	635	0.7846	0.0045	770	0.8245	0.0047
505	0.3430	0.0024	640	0.7869	0.0045	775	0.8246	0.0056
510	0.4036	0.0028	645	0.7893	0.0045	780	0.8266	0.0048

Table 15. Tristimulus values *Y* and chromaticity coordinates *x* and *y*, with expanded uncertainties *U* (*k*=2) for CIE standard illuminant D65 and CIE 1931 standard observer for each color tile, set number NISTCS-XX

Tile	*Y*	*U*	*x*	*U*	*y*	*U*
Black	0.624	0.006	0.3010	0.0011	0.3355	0.0018
Cyan	19.161	0.113	0.1986	0.0000	0.2416	0.0003
Deep Blue	1.119	0.009	0.1994	0.0003	0.1206	0.0008
Deep Gray	5.084	0.029	0.3182	0.0003	0.3356	0.0003
Deep Pink	11.531	0.068	0.4127	0.0004	0.3059	0.0004
Diff Gray	26.181	0.148	0.3140	0.0000	0.3382	0.0000
Diff Green	21.651	0.126	0.2845	0.0002	0.4379	0.0004
Green	21.455	0.125	0.2748	0.0002	0.4236	0.0005
Mid Gray	25.577	0.145	0.3139	0.0000	0.3307	0.0001
Orange	35.184	0.209	0.5228	0.0005	0.3976	0.0005
Pale Gray	62.975	0.357	0.3128	0.0001	0.3301	0.0000
Red	10.086	0.067	0.5850	0.0011	0.3337	0.0005
White	89.994	0.511	0.3141	0.0001	0.3314	0.0001
Yellow	63.350	0.362	0.4467	0.0003	0.4850	0.0002

Table 16. Sources of uncertainty and their standard uncertainty or value for a color tile set, set number NISTCS-XX

Source of Uncertainty	Standard Uncertainty or Value
Signal	
Noise	0.01 % - 0.2 %
Non-linearity	0.2 %
Stray Light	10^{-6}
Wavelength	0.05 nm
Standard	
Random	0.02 %
Systematic	0.2 %

Appendix B

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Uncertainty Analysis for Reflectance Colorimetry

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Abstract

The uncertainty associated with the quantitative description of the color of an object is often necessary for determining the acceptability of that object for its intended application. Uncertainties are also required for establishing the traceability of a measurement to a national metrology institute. A systematic, analytical approach to uncertainty analysis, which conforms to currently accepted practice, is presented for reflectance colorimetry. Two important concepts are stressed – the measurement equation describing the relation between signals and spectral reflectance factor, and correlations both between signals at the same wavelength and between reflectance factors at different wavelengths. The approach is illustrated by considering representative object colors and instrument parameters.

Keywords: colorimetry, correlation, uncertainty

I. Introduction

Determining the uncertainty in the measured color of a specimen has been a topic of interest for many years.[1-9] It has received additional attention with the publication of the *ISO Guide to the Expression of Uncertainty in Measurement*,[10] which describes methods for estimating uncertainties in a consistent manner. Recent publications have applied the principles of this Guide to uncertainty analysis for colorimetry, emphasizing the treatment of correlation.[11,12]

The development of a new reference instrument for reflectance colorimetry at the National Institute of Standards and Technology (NIST) has prompted a detailed analysis of the uncertainties associated with this measurement. From a review of the literature, three important aspects of previous uncertainty analyses for colorimetry became apparent. First, while sources of uncertainty can be caused by either random or systematic effects, most of the previous analyses were restricted to considering only uncertainties caused by random effects.[1,5,6,8,9] Where uncertainties caused by systematic effects were considered, modeling was performed to calculate[2,4] or minimize[7] the effects of these uncertainties. Second, the importance of correlations due to spectral overlap of the color-matching functions was recognized from the beginning,[1,4,5] and has received renewed attention.[9,11,12] Third, the analyses started with a given uncertainty in the spectral reflectance factor,[1,2,4-9] without considering the underlying measurement used to calculate it.

The analysis detailed here presents a systematic, analytical method for calculating uncertainties in reflectance colorimetry and emphasizes two key points. First, the spectral properties of the measurement instrument are important because ratios of signals are used to calculate the spectral reflectance factor of a specimen. Therefore, the measurement equation is used to determine the uncertainty in the spectral reflectance factor. Second, since correlations exist both between signals at the same wavelength and between reflectance factors at different wavelengths, the effects of these correlations are included in the analysis. These concepts are illustrated by considering common sources of uncertainty for a double-grating, single-detector instrument and applying the analysis to representative object colors.

II. Equations for Reflectance Colorimetry

The surface color of a specimen depends upon several factors – the spectral power distribution of the illuminant, the spectral sensitivity of the observer, the geometrical conditions of illumination and observation, and the optical properties of the specimen. Only the last factor depends upon the specimen, and is quantified by the spectral reflectance factor under the given geometrical conditions. Once the spectral reflectance factor is known, the tristimulus values are calculated for a given illuminant and observer, and from these values other quantities are derived, such as chromaticity coordinates or color space values.

The measurement of the spectral reflectance factor of a specimen is performed by comparing signals from the specimen and a standard, under the same measurement conditions. This process is described by the measurement equation

$$R(\lambda_i) = \frac{S(\lambda_i)}{S_s(\lambda_i)} \cdot R_s(\lambda_i)\ , \tag{2.1}$$

where λ_i is the wavelength setting of the instrument, S and S_s are the measured signals from the specimen and standard, respectively, and R and R_s are the reflectance factors for the specimen and standard, respectively. For ease of notation, in the following the wavelength dependence of the signals and reflectance factors will be indicated by subscripts i and j. Therefore, Eq. (2.1) becomes

$$R_i = \frac{S_i}{S_{s,i}} \cdot R_{s,i}\ . \tag{2.2}$$

The tristimulus values X, Y, and Z, for reflectance factors regularly spaced in wavelength, are given by

$$X = \sum_{i=1}^{m} W_{x,i} \cdot R_i\ , \tag{2.3}$$

$$Y = \sum_{i=1}^{m} W_{y,i} \cdot R_i\ ,\ \text{and} \tag{2.4}$$

$$Z = \sum_{i=1}^{m} W_{z,i} \cdot R_i\ , \tag{2.5}$$

where $W_{x,i}$, $W_{y,i}$, and $W_{z,i}$ are the normalized tristimulus weighting factors for a particular illuminant and observer combination and spectral bandwidth and interval.[13] These tristimulus values are then used to calculate chromaticity coordinates, such as x and y or u' and v', or color space values, such as L^*, a^*, and b^* or L^*, u^*, and v^*, as given in Ref. [13].

III. Basics of Uncertainty Analysis

The approach to the uncertainty analysis presented here follows the Guide.[10] This section details the basic definitions and equations used in the uncertainty analysis.

In general, the purpose of a measurement is to determine the value of a measurand y, which is obtained from n other quantities x_k through the functional relationship f, given by

$$y = f(x_1, x_2, \ldots, x_k, \ldots, x_n)\ . \tag{3.1}$$

An example of such a functional relationship, which is used extensively in this paper, is Eq. (2.2), where $R_i = f(S_i, S_{s,i}, R_{s,i}, \lambda)$. The standard uncertainty of an input quantity x_k is the estimated standard deviation associated with this quantity and is denoted by $u(x_k)$. The estimated standard uncertainty in the measurand y is the combined standard uncertainty $u_c(y)$, given by the law of propagation of uncertainty as

$$u_c^2(y) = \sum_{k=1}^{n} \left(\frac{\partial f}{\partial x_k}\right)^2 u^2(x_k) + 2\sum_{k=1}^{n-1} \sum_{l=k+1}^{n} \left(\frac{\partial f}{\partial x_k}\right)\left(\frac{\partial f}{\partial x_l}\right) \cdot u(x_k, x_l)\ . \tag{3.2}$$

Here, $\partial f/\partial x_k$ is the sensitivity coefficient with respect to x_k and $u(x_k, x_l)$ is the covariance of x_k and x_l. The covariance is related to the correlation coefficient $r(x_k, x_l)$ by

$$r(x_k, x_l) = \frac{u(x_k, x_l)}{u(x_k) \cdot u(x_l)}\ , \tag{3.3}$$

where the correlation coefficient is a pure number between –1 and +1, inclusive. For two input quantities that are uncorrelated, $r(x_k, x_l) = 0$, while two quantities that are fully correlated have $r(x_k, x_l) = \pm 1$. In general, sources of uncertainty arising from random and independent effects are uncorrelated, while those arising from systematic effects are correlated. In terms of the correlation coefficients, Eq. (3.2) becomes

$$u_c^2(y) = \sum_{k=1}^{n}\left(\frac{\partial f}{\partial x_k}\right)^2 u^2(x_k) + 2\sum_{k=1}^{n-1}\sum_{l=k+1}^{n}\left(\frac{\partial f}{\partial x_k}\right)\left(\frac{\partial f}{\partial x_l}\right)\cdot r(x_k, x_l)\cdot u(x_k)\cdot u(x_l)\,. \quad (3.4)$$

The covariance, and hence the correlation coefficient, can be calculated using two different techniques, depending on the knowledge of the input quantities x_k and x_l. If the quantities are obtained from coincident experimental data with H values for each quantity, then the covariance is given by

$$u(x_k, x_l) = \frac{1}{H}\sum_{h=1}^{H}(x_{k,h} - \bar{x}_k)(x_{l,h} - \bar{x}_l)\ , \quad (3.5)$$

where $\bar{x}_k$ and $\bar{x}_l$ are the averages of x_k and x_l, respectively. The standard deviations of the quantities are

$$u(x_k) = \sqrt{\frac{1}{H}\sum_{h=1}^{H}(x_{k,h} - \bar{x}_k)^2}\ \text{ and} \quad (3.6)$$

$$u(x_l) = \sqrt{\frac{1}{H}\sum_{h=1}^{H}(x_{l,h} - \bar{x}_l)^2}\ . \quad (3.7)$$

Substituting Eqs. (3.5) to (3.7) into Eq. (3.3) yields the correlation coefficient

$$r(x_k, x_l) = \frac{\sum_{h=1}^{H}(x_{k,h} - \bar{x}_k)(x_{l,j} - \bar{x}_l)}{\sqrt{\sum_{h=1}^{H}(x_{k,h} - x_k)^2 \sum_{l=1}^{H}(x_{l,h} - x_l)^2}}\ . \quad (3.8)$$

In the other technique, analytical expressions for the input quantities are known, so that the quantities are functions of additional variables, given by

$$x_k = g_k(q_1, q_2, \ldots, q_h, \ldots, q_H)\ . \quad (3.9)$$

Then, if $u(q_h)$ is the standard uncertainty associated with the quantity q_h,

$$u^2(x_k) = \sum_{h=1}^{H}\left(\frac{\partial g_k}{\partial q_h}\right)^2 u^2(q_h) + 2\sum_{h=1}^{H-1}\sum_{p=h+1}^{H}\left(\frac{\partial g_k}{\partial q_h}\right)\left(\frac{\partial g_k}{\partial q_p}\right)\cdot r(q_h, q_p)\cdot u(q_h)\cdot u(q_p) \quad \text{and} \quad (3.10)$$

$$u(x_k, x_l) = \sum_{h=1}^{H}\frac{\partial g_k}{\partial q_h}\frac{\partial g_l}{\partial q_h}u^2(q_h) + \sum_{h=1}^{H-1}\sum_{p=h+1}^{H}\left[\left(\frac{\partial g_k}{\partial q_h}\right)\left(\frac{\partial g_l}{\partial q_p}\right) + \left(\frac{\partial g_k}{\partial q_p}\right)\left(\frac{\partial g_l}{\partial q_h}\right)\right]\cdot r(q_h, q_p)\cdot u(q_h)\cdot u(q_p)\,. \quad (3.11)$$

Substitution of Eqs. (3.10) and (3.11) into Eq. (3.3) yields the correlation coefficient $r(x_k, x_l)$. For this technique to work, the correlation coefficients for the additional variables $r(q_h, q_p)$ must be known.

As an example of the second technique, consider a common situation in which the input quantities x_k and x_l are given by

$$x_k = a + \alpha = g_k(a, \alpha) \text{ and} \tag{3.12}$$

$$x_l = b + \beta = g_l(b, \beta) \ , \tag{3.13}$$

where the variables are a, b, α, and β, and only α and β are possibly correlated. The standard uncertainties, using Eq. (3.10) and the sensitivity coefficients from Eqs. (3.12) and (3.13), are

$$u^2(x_k) = 1 \cdot u^2(a) + 0 \cdot u^2(b) + 1 \cdot u^2(\alpha) + 0 \cdot u^2(\beta) = u^2(a) + u^2(\alpha) \text{ and} \tag{3.14}$$

$$u^2(x_l) = 0 \cdot u^2(a) + 1 \cdot u^2(b) + 0 \cdot u^2(\alpha) + 1 \cdot u^2(\beta) = u^2(b) + u^2(\beta) \ . \tag{3.15}$$

The covariance, from Eq. (3.11), is

$$u(x_k, x_l) = (1 \cdot 1 + 0 \cdot 0) \cdot r(\alpha, \beta) \cdot u(\alpha) \cdot u(\beta) \ . \tag{3.16}$$

Substituting Eqs. (3.14) to (3.16) into Eq. (3.3) yields the correlation coefficient

$$r(x_k, x_l) = \frac{r(\alpha, \beta) \cdot u(\alpha) \cdot u(\beta)}{\sqrt{u^2(a) + u^2(\alpha)}\sqrt{u^2(b) + u^2(\beta)}} \ . \tag{3.17}$$

If the only source of uncertainty in Eqs. (3.12) and (3.13) is α and β, so that $u(a) = u(b) = 0$, then $r(x_k, x_l) = r(\alpha, \beta)$. To continue this example further, let the variables α and β be given by

$$\alpha = A \cdot s \text{ and} \tag{3.18}$$

$$\beta = B \cdot s \ , \tag{3.19}$$

where the variables A and B are uncorrelated and the variable s is a common factor. Using Eqs. (3.10) and (3.11), assuming no uncertainty in A and B, and the sensitivity coefficients derived from Eqs. (3.18) and (3.19), yields

$$u^2(\alpha) = A^2 \cdot u^2(s) \ , \tag{3.20}$$

$$u^2(\beta) = B^2 \cdot u^2(s) \ \text{, and} \tag{3.21}$$

$$u(\alpha, \beta) = A \cdot B \cdot u^2(s) \ . \tag{3.22}$$

Therefore,

$$r(\alpha, \beta) = \frac{A \cdot B \cdot u^2(s)}{\sqrt{A^2 \cdot u^2(s)}\sqrt{B^2 \cdot u^2(s)}} = 1 \ . \tag{3.23}$$

IV. Application to Reflectance Colorimetry

A. Overview

As detailed in Section II, the progression from measurement to surface color is spectral reflectance factor, tristimulus values, and chromaticity coordinates or color space values. Therefore, to arrive at the uncertainties in the final values describing the surface color of a specimen, the uncertainties in spectral reflectance factor must be propagated through the calculations. From the measurement equation for the spectral reflectance factor R_i, given by Eq. (2.2), uncertainties in S_i, $S_{s,i}$, $R_{s,i}$ and λ all contribute to an uncertainty in R_i.

Uncertainties in the final color values can be calculated using two different approaches. In the first, the uncertainties in R_i are propagated through to uncertainties in the tristimulus values, which are then used to calculate the uncertainties in the chromaticity coordinates or color space values. In the second approach, Eqs. (2.3) to (2.5) are substituted into the definitions of the final values to obtain equations in terms of R_i. The uncertainties in the final color values given by these equations are calculated directly from the uncertainties in R_i. In both approaches the correlations between the uncertainties in R_i at different wavelengths must be included in the calculations. In addition, if the first approach is used, the correlations between the tristimulus values are also required.

These concepts of propagating uncertainties and taking correlations into account are developed below by considering common sources of uncertainty in R_i[14,15] – signal noise, non-linearity in the signal, and uncertainties in the standard and the wavelength. Signal noise is the result of random processes in both the optical source and detector. Non-linearitys in the signal can arise from several sources; those considered here are an improper zero, mis-alignment of the specimen, and stray-light. An improper zero adds a constant value to all signals, while mis-alignment of the specimen is the result of a difference in location, with respect to the reference plane, between the specimen and the standard. For example, if the specimen and standard are physically different, it may not be possible to align one of the front surfaces with the reference plane. Stray-light is radiant flux that reaches the detector at wavelengths outside the nominal spectral bandwidth of the instrument, which adds a value to each signal. This value depends upon the spectral shape of the illumination, the spectral reflectance of both the specimen and standard, and the responsivity of the receiver. The standard has an uncertainty from its calibration, and there is an uncertainty associated with the wavelength setting of the measuring instrument.

Uncertainties in the normalized tristimulus weighting factors $W_{x,i}$, $W_{y,i}$, and $W_{z,i}$ can be an additional source of uncertainty for reflectance colorimetry. For example, the weighting factors chosen for the calculation may not be appropriate for the spectral bandwidth and interval of the measuring instrument. However, the effect of this source of uncertainty is beyond the scope of this paper. Also, this paper does not address the method for obtaining the uncertainties in the signal, standard, and wavelength, other than to recommend applying the techniques found in the Guide.[10]

In the following, each source of uncertainty – signal noise, signal non-linearity, standard, and wavelength – is considered separately, and the sensitivity coefficients of R_i for each source are obtained using the measurement equation. The correlations between signals at the same wavelength and between reflectance factors at different wavelengths for each of these sources are considered in the analysis.

B. Uncertainty in Spectral Reflectance Factor

The sensitivity coefficients of R_i for the signals S_i and $S_{s,i}$ are

$$\frac{\partial R_i}{\partial S_i} = \frac{R_{s,i}}{S_{s,i}} = \frac{R_i}{S_i} \text{ and} \tag{4.1}$$

$$\frac{\partial R_i}{\partial S_{s,i}} = \frac{-R_{s,i}S_i}{S_{s,i}^2} = \frac{-R_i}{S_{s,i}} \ . \tag{4.2}$$

Substituting these into Eq. (3.4) and dividing by R_i^2 yields the component of standard uncertainty in R_i due to uncertainty in the signals,

$$\frac{u_c^2(R_i)}{R_i^2} = \frac{u^2(S_i)}{S_i^2} + \frac{u^2(S_{s,i})}{S_{s,i}^2} - 2\frac{u(S_i)}{S_i}\frac{u(S_{s,i})}{S_{s,i}} r(S_i, S_{s,i}) \ . \tag{4.3}$$

The correlation coefficient $r(S_i, S_{s,i})$ between the two signals depends upon the source of uncertainty. Since signal noise is a random effect, the standard uncertainties are uncorrelated and $r(S_i, S_{s,i}) = 0$. From Eq. (4.3), the resulting component of standard uncertainty in R_i due to signal noise is

$$\frac{u_c^2(R_i)}{R_i^2} = \frac{u^2(S_i)}{S_i^2} + \frac{u^2(S_{s,i})}{S_{s,i}^2} \ . \tag{4.4}$$

For an non-linearity in the signals, the example given by Eqs. (3.12) and (3.13) and following applies by replacing x_k and x_l by S_i and $S_{s,i}$, respectively. If the non-linearity affects only one of the signals, for example a mis-alignment of the specimen relative to the standard, then $\beta = 0$ and there is no uncertainty in $S_{s,i}$, so Eq. (4.3) becomes

$$\frac{u_c^2(R_i)}{R_i^2} = \frac{u^2(S_i)}{S_i^2} \ . \tag{4.5}$$

If the non-linearity affects both signals, then the correlation coefficient $r(S_i, S_{s,i})$ is needed. For an improper zero, $\alpha = \beta$ since it affects both signals with the same value, so $r(\alpha, \beta) = 1$ and therefore $r(S_i, S_{s,i}) = 1$. For an non-linearity caused by stray-light, the magnitudes of the non-linearity will be different for the two signals because of the different spectral reflectance factors of the specimen and standard. However, the non-linearity can be modeled as Eqs. (3.18) and (3.19) (see Eqs. (5.2) and (5.3)), so $r(\alpha, \beta) = 1$ and hence $r(S_i, S_{s,i}) = 1$. For the non-linearity affecting both signals considered here, where $r(S_i, S_{s,i}) = 1$, Eq. (4.3) becomes

$$\frac{u_c^2(R_i)}{R_i^2} = \left[\frac{u(S_i)}{S_i} - \frac{u(S_{s,i})}{S_{s,i}}\right]^2 \ . \tag{4.6}$$

Note that for the case of an non-linearity that is the same for both signals, Eq. (4.6) implies that if the signals from the specimen and standard are the same, meaning they are similar materials, then the standard uncertainty in R_i is zero.

The sensitivity coefficient of R_i for the spectral reflectance factor of the standard $R_{s,i}$ is

$$\frac{\partial R_i}{\partial R_{s,i}} = \frac{S_i}{S_{s,i}} = \frac{R_i}{R_{s,i}} \ , \tag{4.7}$$

and Eq. (3.4) becomes

$$\frac{u_c^2(R_i)}{R_i^2} = \frac{u^2(R_{s,i})}{R_{s,i}^2} \ . \tag{4.8}$$

Finally, the sensitivity coefficient of R_i for wavelength λ is

$$\frac{\partial R_i}{\partial \lambda} = \frac{\partial \left(S_i / S_{s,i} \right)}{\partial \lambda} R_{s,i} \tag{4.9}$$

and Eq. (3.4) becomes

$$\frac{u_c^2(R_i)}{R_i^2} = \frac{R_{s,i}^2}{R_i^2} \left(\frac{\partial \left(S_i / S_{s,i} \right)}{\partial \lambda} \right)^2 u^2(\lambda) \ . \tag{4.10}$$

Any uncertainty in $R_{s,i}$ due to wavelength is included in Eq. (4.8).

C. Correlations between Wavelengths

The correlation coefficients $r(R_i, R_j)$ for spectral reflectance factors at different wavelengths i and j are calculated for the sources of uncertainty considered here. These correlation coefficients are used in succeeding sections to determine the uncertainty in tristimulus values and chromaticity coordinates and color space values. For all calculations in the following, the signals and spectral reflectance factors are assumed to be positive.

The sources of uncertainty associated with the signals are noise and an non-linearity. Since signal noise is a random effect, there is no correlation between wavelengths, and hence $r(R_i, R_j) = 0$. For an non-linearity, an extension of the approach leading to Eq. (4.6) is used, but now with four signals (from the specimen and the standard at the two wavelengths). If the non-linearity affects only one pair of signals, for example those from the specimen, then $r(R_i, R_j) = 1$. If the non-linearity affects all four signals, as for an improper zero or stray-light, then the correlation coefficient is given by

$$r(R_i, R_j) = \operatorname{sgn}\left(\frac{1}{S_i} - \frac{1}{S_{s,i}} \right) \cdot \operatorname{sgn}\left(\frac{1}{S_j} - \frac{1}{S_{s,j}} \right) \ , \tag{4.11}$$

where $\operatorname{sgn}(x) = +1$ if $x > 0$, -1 if $x < 0$, and 0 if $x = 0$. Equation (4.11) is a result of taking the absolute values of the sensitivity coefficients for the denominator of Eq. (3.3). For the common situation where the standard has a greater reflectance factor than the specimen, $S_{s,i} > S_i$ for all i and $r(R_i, R_j) = +1$ for all i and j. On the other hand, if the standard and specimen have similar spectral reflectance factors, then $r(R_i, R_j)$ can be –1, 0, or +1 depending upon the four signals.

The spectral reflectance factor of the standard, $R_{s,i}$, has uncertainties caused by both random and systematic effects. For the random effects, $r(R_i, R_j) = 0$, while additional analysis is needed for the systematic effects. The spectral reflectance factor of the standard is assigned based upon absolute measurements, which involve ratios of signals and other factors. Therefore, let $R_{s,i}$ be a function of these variables, so that

$$R_{s,i} = f(S_{1,i}, S_{2,i}, \xi) \ , \tag{4.12}$$

where ξ accounts for the other factors that are common to all wavelengths. The sensitivity coefficients of the spectral reflectance factor of the specimen with respect to the variable ξ are

$$\frac{\partial R_i}{\partial \xi} = \frac{\partial R_i}{\partial R_{s,i}} \frac{\partial R_{s,i}}{\partial \xi} = \frac{R_i}{R_{s,i}} \frac{\partial R_{s,i}}{\partial \xi} \text{ and} \tag{4.13}$$

$$\frac{\partial R_j}{\partial \xi} = \frac{\partial R_j}{\partial R_{s,j}} \frac{\partial R_{s,j}}{\partial \xi} = \frac{R_j}{R_{s,j}} \frac{\partial R_{s,j}}{\partial \xi} \ . \tag{4.14}$$

Therefore, the correlation coefficient is given by

$$r(R_i, R_j) = \mathrm{sgn}\left(\frac{\partial R_{s,i}}{\partial \xi}\right) \cdot \mathrm{sgn}\left(\frac{\partial R_{s,j}}{\partial \xi}\right) \ . \tag{4.15}$$

In nearly all cases, this reduces to $r(R_i, R_j) = +1$. For example, for the common 0:45 geometry (illumination angle of 0°, viewing angle of 45°), the spectral reflectance factor of the standard is obtained from signals proportional to the illuminating and reflected radiant flux, S_I and S_R, and from the projected solid angle Ω from the center of the standard to the entrance pupil of the receiver, and is given by

$$R_{s,i} = \frac{S_{R,i}}{S_{I,i}} \frac{1}{\Omega} \ . \tag{4.16}$$

The common factor is Ω, and applying Eq. (4.15) yields $r(R_i, R_j) = +1$.

Finally, uncertainty in the wavelength of the instrument can be correlated between wavelengths. If the uncertainty arises from random effects, then $r(R_i, R_j) = 0$, as usual. However, the uncertainty can also arise from systematic effects. For example, an non-linearity in wavelength may be constant or vary in a systematic manner across the wavelength range of the instrument. The sensitivity coefficients are given by Eq. (4.9), and the correlation coefficient is

$$r(R_i, R_j) = \mathrm{sgn}\left(\frac{\partial \left(S_i / S_{s,i} \right)}{\partial \lambda}\right) \cdot \mathrm{sgn}\left(\frac{\partial \left(S_j / S_{s,j} \right)}{\partial \lambda}\right) \ . \tag{4.17}$$

Therefore, the correlation coefficient for an uncertainty caused by wavelength depends upon the slopes of the signal ratios at the two wavelengths, and can have values of –1, 0, or +1.

The correlation coefficients, both between signals at the same wavelength and between spectral reflectance factors at different wavelengths, are summarized in Table 1 for the common sources of uncertainty considered here.

D. Calculations Based on Tristimulus Values

The uncertainties in spectral reflectance factor, $u(R_i)$ as given in Section IV.B, and their correlations between wavelengths, $r(R_i, R_j)$ as given in Section IV.C, are used to calculate the uncertainty in the tristimulus values. The uncertainties in the tristimulus values are then used to calculate the uncertainty in the chromaticity coordinates or the color space values, taking correlations between tristimulus values into account.

The uncertainty in the tristimulus value X is presented here, and similar considerations apply for Y and Z. For a given source of uncertainty, the uncertainty in X is, from Eq. (3.4), given by

$$u_c^2(X) = \sum_{i=1}^{m}\left(\frac{\partial X}{\partial R_i}\right)^2 u^2(R_i) + 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left(\frac{\partial X}{\partial R_i}\right)\left(\frac{\partial X}{\partial R_j}\right)\cdot r(R_i,R_j)\cdot u(R_i)\cdot u(R_j)\ . \quad (4.18)$$

From Eq. (2.3), the sensitivity coefficients are

$$\frac{\partial X}{\partial R_i} = W_{\mathrm{x},i}\ , \quad (4.19)$$

which, when substituted into Eq. (4.18) yield

$$u_c^2(X) = \sum_{i=1}^{m} W_{\mathrm{x},i}^2 \cdot u^2(R_i) + 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m} W_{\mathrm{x},i}\cdot W_{\mathrm{x},j}\cdot r(R_i,R_j)\cdot u(R_i)\cdot u(R_j)\ . \quad (4.20)$$

If $r(R_i, R_j) = 0$ for all wavelengths, Eq. (4.20) reduces to

$$u_c^2(X) = \sum_{i=1}^{m} W_{\mathrm{x},i}^2 \cdot u^2(R_i)\ , \quad (4.21)$$

while if $r(R_i, R_j) = +1$ for all wavelengths it becomes

$$u_c^2(X) = \left[\sum_{i=1}^{m} W_{\mathrm{x},i}\cdot u(R_i)\right]^2\ . \quad (4.22)$$

However, if $r(R_i, R_j) = -1$ for all wavelengths or depends upon the wavelengths, then Eq. (4.20) does not reduce to a simple form.

The correlations between tristimulus values *X* and *Y* are presented here, and as before similar considerations apply for correlations between *X* and *Z* and between *Y* and *Z*. Substituting Eq. (4.19) and its equivalent for *Y* into Eq. (3.11) yields

$$\begin{aligned} u(X,Y) &= \sum_{i=1}^{m}\frac{\partial X}{\partial R_i}\frac{\partial Y}{\partial R_i}u^2(R_i) \\ &\quad + \sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left[\frac{\partial X}{\partial R_i}\frac{\partial Y}{\partial R_j} + \frac{\partial X}{\partial R_j}\frac{\partial Y}{\partial R_i}\right]\cdot r(R_i,R_j)\cdot u(R_i)\cdot u(R_j) \\ &= \sum_{i=1}^{m} W_{\mathrm{x},i}\cdot W_{\mathrm{y},i}\cdot u^2(R_i) \\ &\quad + \sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left[W_{\mathrm{x},i}\cdot W_{\mathrm{y},j} + W_{\mathrm{x},j}\cdot W_{\mathrm{y},i}\right]\cdot r(R_i,R_j)\cdot u(R_i)\cdot u(R_j)\ . \end{aligned} \quad (4.23)$$

Substituting Eq. (4.23) and the square roots of Eq. (4.20) and its equivalent for *Y* into Eq. (3.3) yields the correlation coefficient between *X* and *Y*,

$$r(X,Y) = \frac{u(X,Y)}{u(X)\cdot u(Y)}\ . \quad (4.24)$$

Note that $r(X, Y)$ can have values between –1 and +1, depending on the values of $r(R_i, R_j)$, $u(R_i)$, and $u(R_j)$, and hence is a function of the source of uncertainty.

The uncertainties in chromaticity coordinates and color space values are obtained from their dependence on the tristimulus values. Let Γ represent either a chromaticity coordinate or a color space value. Using Eq. (3.4) with $x_k = X$, Y, or Z, the combined uncertainty from each source is given by

$$u_c^2(\Gamma) = \left(\frac{\partial\Gamma}{\partial X}\right)^2 u^2(X) + \left(\frac{\partial\Gamma}{\partial Y}\right)^2 u^2(Y) + \left(\frac{\partial\Gamma}{\partial Z}\right)^2 u^2(Z)$$
$$+ 2\left(\frac{\partial\Gamma}{\partial X}\right)\left(\frac{\partial\Gamma}{\partial Y}\right)\cdot r(X,Y)\cdot u(X)\cdot u(Y)$$
$$+ 2\left(\frac{\partial\Gamma}{\partial X}\right)\left(\frac{\partial\Gamma}{\partial Z}\right)\cdot r(X,Z)\cdot u(X)\cdot u(Z) \quad (4.25)$$
$$+ 2\left(\frac{\partial\Gamma}{\partial Y}\right)\left(\frac{\partial\Gamma}{\partial Z}\right)\cdot r(Y,Z)\cdot u(Y)\cdot u(Z)\,.$$

The sensitivity coefficients for common chromaticity coordinates and color space values are given in Appendix A, while the standard uncertainties $u(X)$, $u(Y)$, and $u(Z)$ are given by Eq. (4.18) and its equivalents, and the correlation coefficients $r(X, Y)$, $r(X, Z)$ and $r(Y, Z)$ are given by Eq. (4.24) and its equivalents. An interesting result for the chromaticity coordinates x and y is that, if the standard uncertainty is a constant proportion of the reflectance factor at all wavelengths, and the correlation coefficient between wavelengths is +1, then the uncertainty in x and y is zero. This is usually the case for an uncertainty in the standard caused by systematic effects.

The uncertainties in chroma C and hue h can be derived is a similar fashion. Using the L^*, a^*, b^* color space as an example, the chroma C_{ab}^* is given by

$$C_{ab}^* = \sqrt{(a^*)^2 + (b^*)^2} \quad (4.26)$$

and the combined uncertainty in chroma is given by

$$u_c^2(C_{ab}^*) = \left(\frac{\partial C_{ab}^*}{\partial a^*}\right)^2 u^2(a^*) + \left(\frac{\partial C_{ab}^*}{\partial b^*}\right)^2 u^2(b^*) \quad (4.27)$$
$$+ 2\left(\frac{\partial C_{ab}^*}{\partial a^*}\right)\left(\frac{\partial C_{ab}^*}{\partial b^*}\right)\cdot r(a^*,b^*)\cdot u(a^*)\cdot u(b^*)\,.$$

A similar equation applies for h_{ab}^*. The correlation coefficient $r(a^*, b^*)$ is given by

$$r(a^*,b^*) = \frac{u(a^*,b^*)}{u(a^*)\cdot u(b^*)}\ , \quad (4.28)$$

where $u(a^*)$ and $u(b^*)$ are given by Eq. (4.25) and $u(a^*, b^*)$, from Eq. (3.11), is given by

$$u(a^*,b^*) = \frac{\partial a^*}{\partial Y}\frac{\partial b^*}{\partial Y}u^2(Y)$$
$$+ \left[\frac{\partial a^*}{\partial X}\frac{\partial b^*}{\partial Y} + \frac{\partial a^*}{\partial Y}\frac{\partial b^*}{\partial X}\right]\cdot r(X,Y)\cdot u(X)\cdot u(Y)$$
$$+ \left[\frac{\partial a^*}{\partial X}\frac{\partial b^*}{\partial Z} + \frac{\partial a^*}{\partial Z}\frac{\partial b^*}{\partial X}\right]\cdot r(X,Z)\cdot u(X)\cdot u(Z) \quad (4.29)$$
$$+ \left[\frac{\partial a^*}{\partial Y}\frac{\partial b^*}{\partial Z} + \frac{\partial a^*}{\partial Z}\frac{\partial b^*}{\partial Y}\right]\cdot r(Y,Z)\cdot u(Y)\cdot u(Z)\,.$$

Note that the correlation coefficient $r(a^*, b^*)$ applies to both C_{ab}^* and h_{ab}^*.

E. Calculations Based on Spectral Reflectance Factors

The chromaticity coordinates and color space values can also be calculated directly from the spectral reflectance factor by substituting Eqs. (2.3) to (2.5) into their definitions. The uncertainties in the chromaticity coordinates and color space values are then calculated from the uncertainties in the spectral reflectance factor using Eq. (3.4). The sensitivity coefficients in terms of the spectral reflectance factor are obtained by applying the chain rule, so again letting Γ represent either a chromaticity coordinate or a color space value

$$\frac{\partial \Gamma}{\partial R_i} = \frac{\partial \Gamma}{\partial X}\frac{\partial X}{\partial R_i} + \frac{\partial \Gamma}{\partial Y}\frac{\partial Y}{\partial R_i} + \frac{\partial \Gamma}{\partial Z}\frac{\partial Z}{\partial R_i} \quad . \tag{4.30}$$

The derivatives with respect to the tristimulus values are given in Appendix A. Using Eq. (4.30) with Eq. (3.4) yields the combined uncertainty in Γ for each source of uncertainty,

$$u_{\mathrm{c}}^2(\Gamma) = \sum_{i=1}^{m}\left(\frac{\partial \Gamma}{\partial R_i}\right)^2 u^2(R_i) + 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left(\frac{\partial \Gamma}{\partial R_i}\right)\left(\frac{\partial \Gamma}{\partial R_j}\right)\cdot r(R_i, R_j)\cdot u(R_i)\cdot u(R_j)\,. \tag{4.31}$$

The uncertainties in chroma and hue in terms of uncertainties in the spectral reflectance factor are also obtained by applying the chain rule. Using the example of $C_{\mathrm{ab}}*$,

$$\frac{\partial C_{\mathrm{ab}}*}{\partial R_i} = \frac{\partial C_{\mathrm{ab}}*}{\partial a*}\frac{\partial a*}{\partial R_i} + \frac{\partial C_{\mathrm{ab}}*}{\partial b*}\frac{\partial b*}{\partial R_i} \quad , \tag{4.32}$$

where $\partial a*/\partial R_i$ and $\partial b*/\partial R_i$ are given by Eq. (4.30).

F. Summary

A step-by-step summary of the procedure for analyzing uncertainties in reflectance colorimetry is presented below. The relevant equations and sections for each step are given in brackets. The variable Γ below represents the final value, either a chromaticity coordinate such as *u'* or *v'* or a color space value such as *L**, *a**, or *b**.

1. Identify all independent sources of uncertainty.
2. Assign standard uncertainties to these sources, as described in the Guide.
3. Calculate the standard uncertainty in spectral reflectance factor, $u(R_i)$, for each source of uncertainty, using the measurement equation and taking any correlations between signals at the same wavelength into account with the correlation coefficient $r(S_i, S_{\mathrm{s},i})$. [Eq. (2.2) and Section IV.B]
4. Calculate the correlation coefficient between spectral reflectance factors at different wavelengths, $r(R_i, R_j)$, for each source of uncertainty. [Section IV.C]
5. If using the tristimulus values to calculate Γ
   a. Calculate the uncertainties in the tristimulus values based on $u(R_i)$ and $r(R_i, R_j)$ from steps 3 and 4 for each source of uncertainty. [Eq. (4.18)]
   b. Calculate the correlation coefficients between the tristimulus values for each source of uncertainty. [Eq. (4.24)]
   c. Calculate the sensitivity coefficients for Γ with respect to the tristimulus values, $\partial\Gamma/\partial X$, $\partial\Gamma/\partial Y$, and $\partial\Gamma/\partial Z$. [Appendix A]

d. Calculate the uncertainty in Γ using the results from steps a, b, and c for each source of uncertainty. [Eq. (4.25)]

6. If using the spectral reflectance factor to calculate Γ
   a. Calculate the sensitivity coefficient for Γ with respect to R_i. [Eq. (4.30) and Appendix A]
   b. Calculate the uncertainty in Γ using the results from steps 3 and 4 for each source of uncertainty. [Eq. (4.31)]
7. Calculate the final uncertainty in Γ using the root-sum-square of the uncertainties from all the sources obtained in step 5.d or 6.b.

V. Example Calculations

The general concepts of uncertainty analysis for reflectance colorimetry detailed above are applied to an example. The uncertainties in the L^*, a^*, b^* color space values from the common sources of uncertainty considered above for four representative specimens are calculated for the Commission Internationale de l'Eclairage (CIE) D65 Standard Illuminant and the 1964 Standard Colorimetric Observer.[16] The signals used in the calculations are taken from measurements on a reference instrument. The instrument consists of a quartz-tungsten-halogen lamp, a monochromator illuminator, and a silicon photodiode detector, the geometry of measurement is 0:45, and the wavelength increment and spectral bandwidth were both 5 nm. While the uncertainties calculated below are specific to the specimens and instrument, the purpose of this example is to illustrate the uncertainty analysis so that it can be more easily applied to other specimens and instruments.

The spectral reflectance factors of the four representative specimens and the standard are shown in Fig. 1, along with designations based upon their color. These designations will be used for the remainder of this section. The standard was Spectralon[*], which has a nearly constant reflectance factor over the wavelength range. The gray specimen is spectrally neutral, while the red specimen has a reflectance factor that is small at short wavelengths and then increases rapidly to become large at long wavelengths. The green and deep blue specimens have maxima of their reflectance factors at different wavelengths. The wavelength range in Fig. 1 extends past the limits for color calculations, 380 nm to 780 nm, because stray-light contributes to the signal from all wavelengths at which the detector is sensitive, in this case as long as 1100 nm.

The weighting factors for the D65 Illuminant and the 1964 Observer are shown in Fig. 2. The signals from the instrument when measuring the Spectralon standard are shown in Fig. 3 as a function of wavelength. The features in the signal at wavelengths of 460 nm and 750 nm are due to a change of the order-sorting filter. From the measurement equation, Eq. (2.2), since the reflectance factor of the standard is nearly constant, the signals from the specimen are essentially the reflectance factors multiplied by the signal shown in Fig. 3.

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[*] Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Following the first two steps in Section IV.F, the sources of uncertainty are the same as those considered above and listed in Table 1. The standard uncertainties for each source are chosen to be representative of a high-quality instrument. The uncertainty due to noise in the signals is a constant 0.1 % for both the specimen and the standard, so

$$\frac{u(S_i)}{S_i} = \frac{u(S_{s,i})}{S_{s,i}} = 0.001 \ . \tag{5.1}$$

The uncertainty due to an non-linearity of the specimen affects only the signal from the specimen, and is also a constant 0.1 %. The uncertainty due to stray-light affects both the specimen and standard signals. The uncertainty is modeled by

$$u(S_i) = \sum_i S_i \cdot 10^{-N} \quad \text{and} \tag{5.2}$$

$$u(S_{s,i}) = \sum_i S_{s,i} \cdot 10^{-N} \ , \tag{5.3}$$

where N is the stray-light rejection, taken to be $N = 6$ for this example. The uncertainty due to wavelength is $u(\lambda) = 0.1$ nm across the entire wavelength range. The uncertainty in the reflectance factor of the standard due to random effects is 0.02 %, while the uncertainty due to systematic effects is 0.2 %. These uncertainties for the standard are typical of those from a national metrology institute.[17]

The third step in Section IV.F is to calculate the standard uncertainty in the spectral reflectance factor for each source of uncertainty. Using Eq. (5.1) for the uncertainty in the signals due to noise, and Eq. (4.4), the standard uncertainty in the reflectance factor is

$$\frac{u_c(R_i)}{R_i} = \sqrt{(0.001)^2 + (0.001)^2} = 0.0014 \ . \tag{5.4}$$

For an uncertainty due to an non-linearity affecting only the signal from the specimen, Eq. (4.5) is applicable, and so

$$\frac{u_c(R_i)}{R_i} = 0.001 \ . \tag{5.5}$$

However, for an uncertainty due to stray-light, which affects both signals, Eq. (4.6) is applicable, so combining this with Eqs. (5.2) and (5.3) and taking the positive square root yields

$$\frac{u_c(R_i)}{R_i} = 10^{-6} \left| \frac{\sum S_i}{S_i} - \frac{\sum S_{s,i}}{S_{s,i}} \right| \ . \tag{5.6}$$

For an uncertainty due to wavelength, Eq. (4.10) applies, and so

$$\frac{u_c(R_i)}{R_i} = \frac{R_{s,i}}{R_i} \left| \frac{\partial \left(S_i / S_{s,i} \right)}{\partial \lambda} \cdot 0.1\text{nm} \right| . \tag{5.7}$$

For the uncertainties in the standard due to both random and systematic effects, Eq. (4.8) applies, so

$$\frac{u_c(R_i)}{R_i} = 0.0002 \tag{5.8}$$

for the random effects and

$$\frac{u_c(R_i)}{R_i} = 0.002 \tag{5.9}$$

for the systematic effects.

The fourth step in Section IV.F is to calculate the correlation coefficient between spectral reflectance factors at different wavelengths for each source of uncertainty. These are given in Table 1. The fifth and sixth steps are to calculate the uncertainties in L^*, a^*, and b^* from either the tristimulus values or directly from the spectral reflectance factors. Both approaches are presented here.

Given the uncertainties in spectral reflectance factor and their correlations for each source of uncertainty, and the weighting factors for the Illuminant and Observer, the uncertainties in the tristimulus values are given by Eq. (4.20) for X and its equivalent for Y and Z. The correlation coefficients between tristimulus values are given by Eqs. (4.23) and (4.24) for X, with similar equations for Y and Z. For uncertainties due to systematic effects (those with $r(R_i, R_j) = -1$ or $+1$), the correlation coefficients are identically one. The correlation coefficients for uncertainties due to random effects are given in Table 2 for each specimen. Referring to Figs. 1 and 2, the correlation coefficient for X and Y is largest for all the colors in Table 2 because these weighting functions have the most overlap with each other. This behavior is enhanced for the red specimen because the reflectance factor is small for wavelengths shorter than 600 nm.

The uncertainties in L^*, a^*, and b^* are calculated using Eq. (4.25). The sensitivity coefficients $\partial L^*/\partial Y$, $\partial a^*/\partial X$, $\partial a^*/\partial Y$, $\partial b^*/\partial Y$, and $\partial b^*/\partial Z$ are given by Eqs. (A.13) to (A.17), the uncertainties in the tristimulus values $u(X)$, $u(Y)$, and $u(Z)$ are given by Eq. (4.20) and its equivalents, and the correlation coefficients between the tristimulus values $r(X, Y)$, $r(X, Z)$ and $r(Y, Z)$ are either +1 for uncertainties caused by systematic effects or are given in Table 2 for uncertainties caused by random effects. For example, L^* is a function only of Y, so the uncertainty in L^* is given by

$$u_c^2(L^*) = \left[\frac{116}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]^2 u^2(Y) \tag{5.10}$$

while a^* is a function of X and Y so the uncertainty in a^* is given by

$$u_c^2(a^*) = \left[\frac{500}{3}\left(\frac{1}{X^2 X_n}\right)^{1/3}\right]^2 u^2(X) + \left[\frac{-500}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]^2 u^2(Y) - 2\cdot\frac{500}{3}\cdot\frac{500}{3}\left(\frac{1}{X^2 X_n}\right)^{1/3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3} r(X,Y)\cdot u(X)\cdot u(Y)\,. \tag{5.11}$$

The uncertainties in C_{ab}^* and h_{ab}^* are calculated using Eq. (4.27) and its equivalent for h_{ab}^* and the uncertainties $u(a^*)$ and $u(b^*)$ given by the procedure detailed in the previous paragraph. The correlation coefficient $r(a^*, b^*) = -1$ or $+1$ for uncertainties caused by systematic effects, and is given in Table 2 for uncertainties caused by random effects. The sensitivity coefficients $\partial C_{ab}^*/\partial a^*$, $\partial C_{ab}^*/\partial b^*$, $\partial h_{ab}^*/\partial a^*$, and $\partial h_{ab}^*/\partial b^*$ are given by Eqs. (A.18) to (A.21). For example, the uncertainty in C_{ab}^* is given by

$$u_c^2(C_{ab}^*) = \left(\frac{a^*}{C_{ab}^*}\right)^2 u^2(a^*) + \left(\frac{b^*}{C_{ab}^*}\right)^2 u^2(b^*)$$
$$+ 2\cdot\left(\frac{a^*}{C_{ab}^*}\right)\left(\frac{b^*}{C_{ab}^*}\right)\cdot r(a^*,b^*)\cdot u(a^*)\cdot u(b^*)\,. \tag{5.12}$$

To calculate the uncertainties is L^*, a^*, and b^* directly from the spectral reflectance factors, Eq. (4.31) is used. The sensitivity coefficients are given by Eq. (4.30) using Eqs. (A.13) to (A.17) and (4.19). For example, the sensitivity coefficients for L^* are given by

$$\frac{\partial L^*}{\partial R_i} = \left[\frac{116}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]\cdot W_{y,i}\ , \tag{5.13}$$

for a^* by

$$\frac{\partial a^*}{\partial R_i} = \left[\frac{500}{3}\left(\frac{1}{X^2 X_n}\right)^{1/3}\right]\cdot W_{x,i} + \left[\frac{-500}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]\cdot W_{y,i}\ , \tag{5.14}$$

and for C_{ab}^* by

$$\frac{\partial C_{ab}^*}{\partial R_i} = \left(\frac{a^*}{C_{ab}^*}\right)\cdot\left\{\left[\frac{500}{3}\left(\frac{1}{X^2 X_n}\right)^{1/3}\right]\cdot W_{x,i} + \left[\frac{-500}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]\cdot W_{y,i}\right\}$$
$$+ \left(\frac{b^*}{C_{ab}^*}\right)^2\cdot\left\{\left[\frac{200}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]\cdot W_{y,i} + \left[\frac{-200}{3}\left(\frac{1}{Z^2 Z_n}\right)^{1/3}\right]\cdot W_{z,i}\right\}. \tag{5.15}$$

The uncertainties in the values are given by substituting the appropriate equation from Eqs. (5.13) to (5.15) into Eq. (4.31). Using L^* as an example, this results in

$$u_c^2(L^*) = \sum_{i=1}^{m}\left[\frac{116}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\cdot W_{y,i}\right]^2 u^2(R_i)$$
$$+ 2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left[\frac{116}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3}\right]^2\cdot W_{y,i}\cdot W_{y,j}\cdot r(R_i,R_j)\cdot u(R_i)\cdot u(R_j)\,, \tag{5.16}$$

where $u(R_i)$, $u(R_j)$, and $r(R_i, R_j)$ are the uncertainties and correlation coefficients appropriate to the source of uncertainty.

The absolute uncertainties (k = 1) in the color scale values L^*, a^*, and b^* from each source of uncertainty considered here are shown in Fig. 4 for the four representative specimens. Note that the vertical scale for the red specimen is three times that of the other specimens. Several conclusions can be drawn from the results presented in Fig. 4. Signal noise contributes uncertainty for all the specimens, with the uncertainties in a^* and b^* larger than that of L^*. The effect of correlation is also apparent. Even though the uncertainties due to noise and non-linearity are both 0.1 % of the signal, the former is uncorrelated between wavelengths, while the later is correlated. This results in the uncertainty in L^* being larger for the correlated uncertainty and the uncertainties in a^*

and b^* being smaller. The uncertainties caused by random effects in the standard are simply reduced in magnitude from those caused by signal noise.

The uncertainties caused by systematic effects in the standard are significant for all the specimens, and can be the largest source of uncertainty for those specimens with nearly constant reflectance factor over the visible wavelength region. The uncertainties caused by wavelength and stray-light also depend on the spectral shape of the reflectance factor. The largest uncertainties due to wavelength are for the red specimen, whose reflectance factor increases rapidly with wavelength. The reflectance factors of the deep blue and green specimens also depend upon wavelength, but the slope of the reflectance factor, and hence the sensitivity coefficients, changes sign several times over the wavelength range. In addition, the reflectance factor of the deep blue specimen is nearly constant over much of the visible wavelength range. The uncertainty due to stray-light is largest for the red specimen because of the combination of the spectral reflectance factor of this color, shown in Fig. 1, and the radiant flux illuminating the specimen, which is proportional to the signal in Fig. 3. Since the reflectance factor is small over the wavelength range where the flux is also low, while both are large at longer wavelengths, there is a significant stray-light contribution to the signals at short wavelengths and hence a contribution to the uncertainty in L^*, a^*, and b^*. Finally, the uncertainties are smallest for those specimens with a spectral reflectance factor similar to that of the standard, namely gray, while the uncertainties are largest for those specimens that are most dissimilar.

The results shown in Fig. 4 are not sensitive to the Standard Illuminant or Observer chosen for the analysis, provided an illuminant with sharp spectral features at only one or a few wavelengths is not used. Also, the uncertainties are proportional to the magnitudes of uncertainties of the sources. If the uncertainty for one of the sources is increased by a factor of ten, then the corresponding uncertainty shown in Fig. 4 is also increased by a factor of ten. The combined uncertainty in L^*, a^*, or b^* is the root-sum-square of the uncertainties due to all the sources. For example, for the red specimen, the combined uncertainty in b^* is $u_c(b^*) = [0.010^2 + 0.012^2 + 0.284^2 + 0.071^2 + 0.001^2 + 0.024^2]^{1/2} = 0.294$. The expanded uncertainty of b^*, with a coverage factor $k = 2$, is 0.588.

VI. Summary

Uncertainties in reflectance colorimetry are important, and have received attention over the years. Application of the *ISO Guide to the Expression of Uncertainty in Measurement* allows the uncertainties to be calculated using a systematic, analytical approach. This requires consideration of the measurement equation, relating signals to spectral reflectance factor, and correlations both between signals at the same wavelength and between reflectance factors at different wavelengths. This approach was detailed for common sources of uncertainty and applied to representative object colors and instrument parameters.

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Appendix A. Sensitivity coefficients for common chromaticity coordinates and color space values

1. Chromaticity coordinates
   a. *x*, *y*

$$\frac{\partial x}{\partial X} = \frac{Y + Z}{(X + Y + Z)^2} \tag{A.1}$$

$$\frac{\partial x}{\partial Y} = \frac{-X}{(X + Y + Z)^2} \tag{A.2}$$

$$\frac{\partial x}{\partial Z} = \frac{-X}{(X + Y + Z)^2} \tag{A.3}$$

$$\frac{\partial y}{\partial X} = \frac{-Y}{(X + Y + Z)^2} \tag{A.4}$$

$$\frac{\partial y}{\partial Y} = \frac{X + Z}{(X + Y + Z)^2} \tag{A.5}$$

$$\frac{\partial y}{\partial Z} = \frac{-Y}{(X + Y + Z)^2} \tag{A.6}$$

   b. *u'*, *v'*

$$\frac{\partial u'}{\partial X} = \frac{60Y + 12Z}{(X + 15Y + 3Z)^2} \tag{A.7}$$

$$\frac{\partial u'}{\partial Y} = \frac{-60X}{(X + 15Y + 3Z)^2} \tag{A.8}$$

$$\frac{\partial u'}{\partial Z} = \frac{-12X}{(X + 15Y + 3Z)^2} \tag{A.9}$$

$$\frac{\partial v'}{\partial X} = \frac{-9Y}{(X + 15Y + 3Z)^2} \tag{A.10}$$

$$\frac{\partial v'}{\partial Y} = \frac{9X + 27Z}{(X + 15Y + 3Z)^2} \tag{A.11}$$

$$\frac{\partial v'}{\partial Z} = \frac{-27Y}{(X + 15Y + 3Z)^2} \tag{A.12}$$

2. Color space values
   a. *L**, *a**, *b**

$$\frac{\partial L^*}{\partial Y} = \frac{116}{3}\left(\frac{1}{Y^2 Y_n}\right)^{1/3} \tag{A.13}$$

$$\frac{\partial a^*}{\partial X} = \frac{500}{3}\left(\frac{1}{X^2 X_\mathrm{n}}\right)^{1/3} \tag{A.14}$$

$$\frac{\partial a^*}{\partial Y} = \frac{-500}{3}\left(\frac{1}{Y^2 Y_\mathrm{n}}\right)^{1/3} \tag{A.15}$$

$$\frac{\partial b^*}{\partial Y} = \frac{200}{3}\left(\frac{1}{Y^2 Y_\mathrm{n}}\right)^{1/3} \tag{A.16}$$

$$\frac{\partial b^*}{\partial Z} = \frac{-200}{3}\left(\frac{1}{Z^2 Z_\mathrm{n}}\right)^{1/3} \tag{A.17}$$

$$\frac{\partial C_\mathrm{ab}^*}{\partial a^*} = \frac{a^*}{C_\mathrm{ab}^*} \tag{A.18}$$

$$\frac{\partial C_\mathrm{ab}^*}{\partial b^*} = \frac{b^*}{C_\mathrm{ab}^*} \tag{A.19}$$

$$\frac{\partial h_\mathrm{ab}^*}{\partial a^*} = \frac{-b^*}{(C_\mathrm{ab}^*)^2} \tag{A.20}$$

$$\frac{\partial h_\mathrm{ab}^*}{\partial b^*} = \frac{a^*}{(C_\mathrm{ab}^*)^2} \tag{A.21}$$

b. *L**, *u**, *v**

$$\frac{\partial L^*}{\partial Y} = \frac{116}{3}\left(\frac{1}{Y^2 Y_\mathrm{n}}\right)^{1/3} \tag{A.22}$$

$$\frac{\partial u^*}{\partial X} = 13L^* \cdot \frac{60Y + 12Z}{(X + 15Y + 3Z)^2} \tag{A.23}$$

$$\frac{\partial u^*}{\partial Y} = 13\frac{116}{3}\left(\frac{1}{Y^2 Y_\mathrm{n}}\right)^{1/3}(u' - u'_\mathrm{n}) + 13L^* \cdot \frac{-60X}{(X + 15Y + 3Z)^2} \tag{A.24}$$

$$\frac{\partial u^*}{\partial Z} = 13L^* \cdot \frac{-12X}{(X + 15Y + 3Z)^2} \tag{A.25}$$

$$\frac{\partial v^*}{\partial X} = 13L^* \cdot \frac{-9Y}{(X + 15Y + 3Z)^2} \tag{A.26}$$

$$\frac{\partial v^*}{\partial Y} = 13\frac{116}{3}\left(\frac{1}{Y^2 Y_\mathrm{n}}\right)^{1/3}(v' - v'_\mathrm{n}) + 13L^* \cdot \frac{9X + 27Z}{(X + 15Y + 3Z)^2} \tag{A.27}$$

$$\frac{\partial v^*}{\partial Z} = 13L^* \cdot \frac{-27Y}{(X + 15Y + 3Z)^2} \tag{A.28}$$

$$\frac{\partial C_{uv}^*}{\partial u^*} = \frac{u^*}{C_{uv}^*} \tag{A.29}$$

$$\frac{\partial C_{uv}*}{\partial v*} = \frac{v*}{C_{uv}*} \tag{A.30}$$

$$\frac{\partial h_{uv}*}{\partial u*} = \frac{-v*}{\left(C_{uv}*\right)^2} \tag{A.31}$$

$$\frac{\partial h_{uv}*}{\partial v*} = \frac{u*}{\left(C_{uv}*\right)^2} \tag{A.32}$$

Tables

Table 1. Correlation coefficients for common sources of uncertainty

	Correlation Coefficient	
Source of Uncertainty	$r(S_i, S_{s,i})$	$r(R_i, R_j)$
Signal		
Noise	0	0
Non-linearity		
One signal	--	+1
Two signals	+1	+1 [a] [Eq. (4.11)]
Standard		
Random effects	--	0
Systematic effects	--	+1 [b] [Eq. (4.15)]
Wavelength	--	–1, 0, or +1 [Eq. (4.17)]

Notes:

[a] $r(R_i, R_j) = +1$ if $S_{s,i} > S_i$ or $S_{s,i} < S_i$ for all wavelengths i. Otherwise, $r(R_i, R_j) = -1$, 0, or +1 depending on the magnitudes of the signals.

[b] +1 in nearly all cases

Table 2. Correlation coefficients between tristimulus values and a^* and b^* due to uncertainties caused by random effects

Correlation Coefficient	Specimen Color			
	Gray	Deep Blue	Green	Red
$r(X, Y)$	0.7746	0.7289	0.7299	0.9648
$r(X, Z)$	0.2957	0.3070	0.2299	0.0281
$r(Y, Z)$	0.1381	0.1549	0.1850	0.0330
$r(a^*, b^*)$	-0.4215	-0.3653	-0.4344	0.5539

Figure Captions

Figure 1. Reflectance factor as a function of wavelength for the example specimens and the standard. The colors of the specimens are indicated.

Figure 2. Weighting factors as a function of wavelength for the D65 Illuminant and 1964 Observer.

Figure 3. Signal as a function of wavelength when measuring the standard.

Figure 4. Absolute uncertainties ($k = 1$) in the L^*, a^*, b^* color scale values caused by the indicated sources of uncertainty for the example specimens. The sources of uncertainty are noise in the signals, an non-linearity of the specimen signals, stray-light contribution to the signals, the wavelength of the instrument (WL), and the reflectance factor of the standard (Std) caused by random (R) and systematic (S) effects.

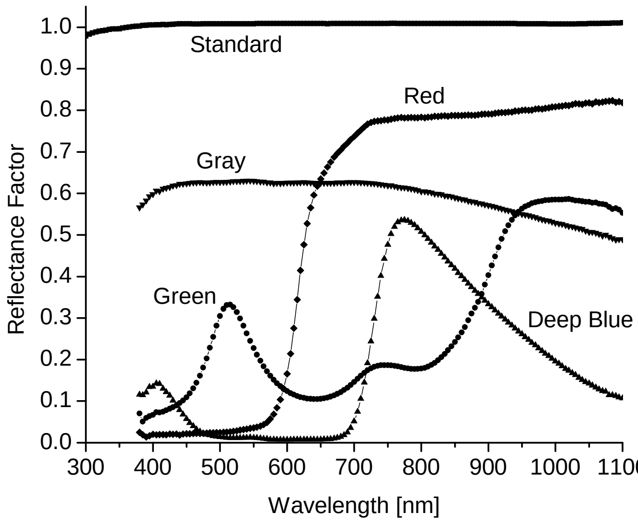


Figure 1.

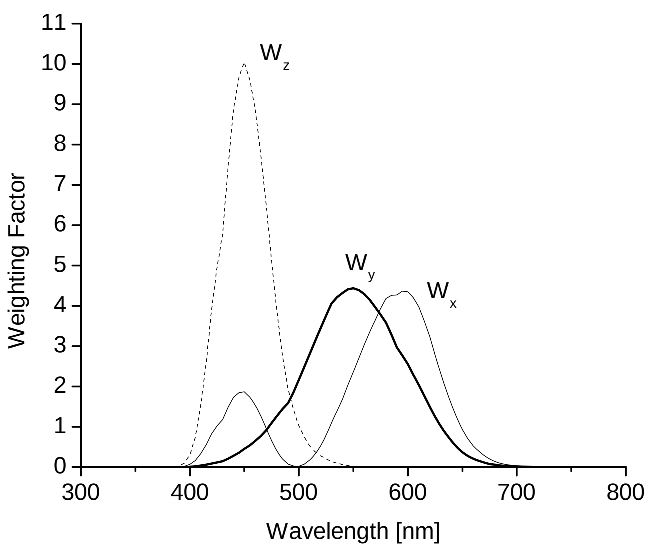
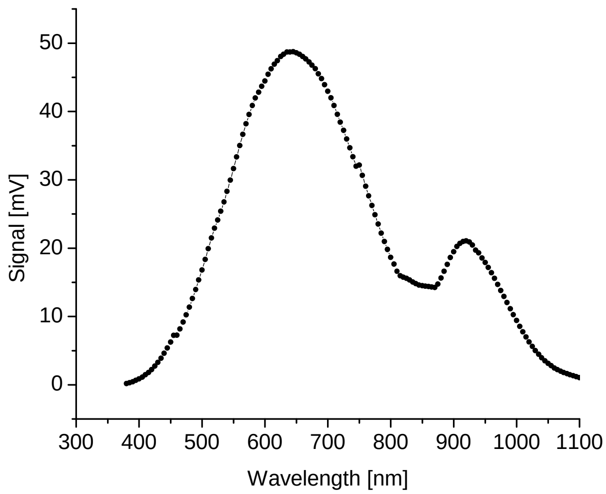


Figure 2.



50
40
30
20
10
0
Signal [mV]
300
400
500
600
700
800
900
1000
1100
Wavelength [nm]

Figure 3.

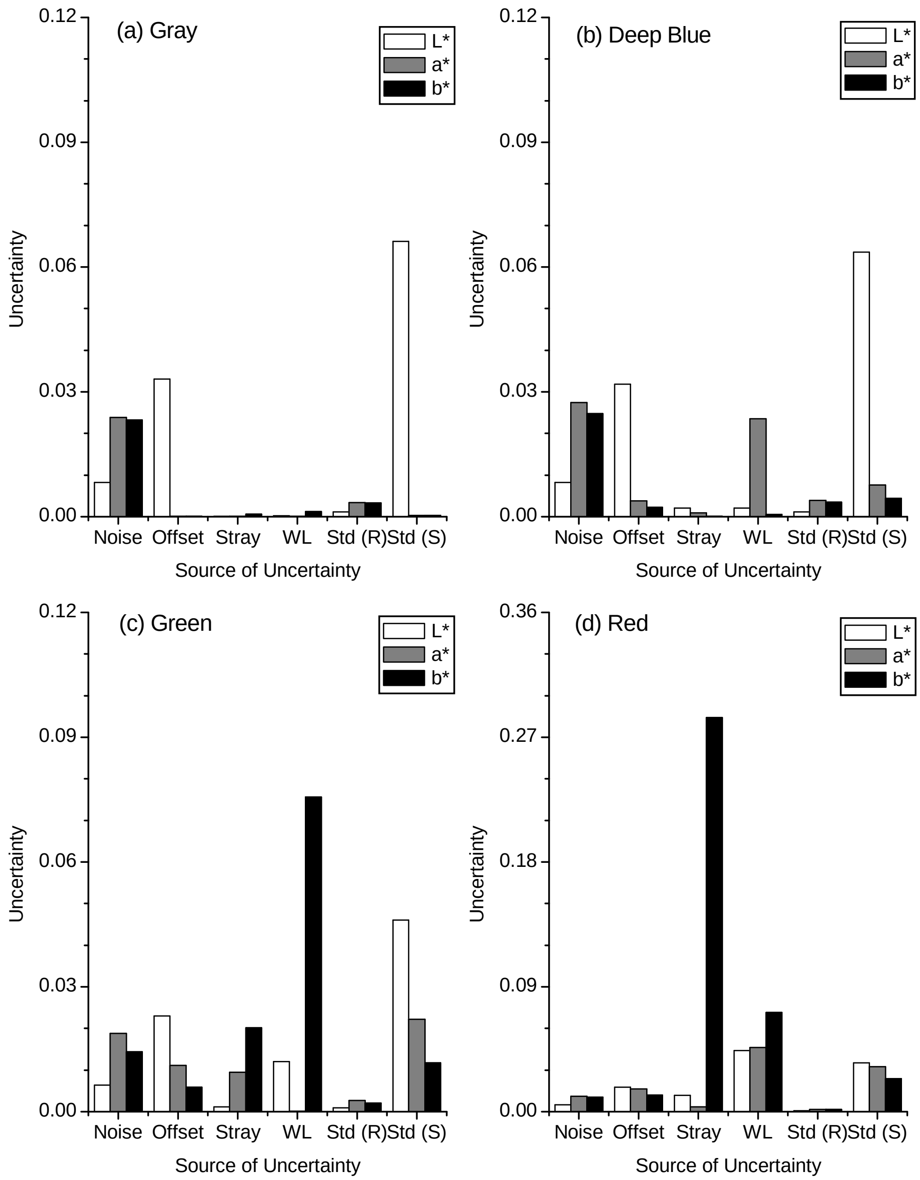

(a) Gray
(b) Deep Blue
(c) Green
(d) Red
L*
a*
b*
Uncertainty
Source of Uncertainty
Noise
Offset
Stray
WL
Std (R)
Std (S)
0.00
0.03
0.06
0.09
0.12
0.18
0.27
0.36

Figure 4.