Uncertainty Evaluation in Reflectance Colorimetry

Maria Nadal

NIST

Measurement Uncertainty Workshop

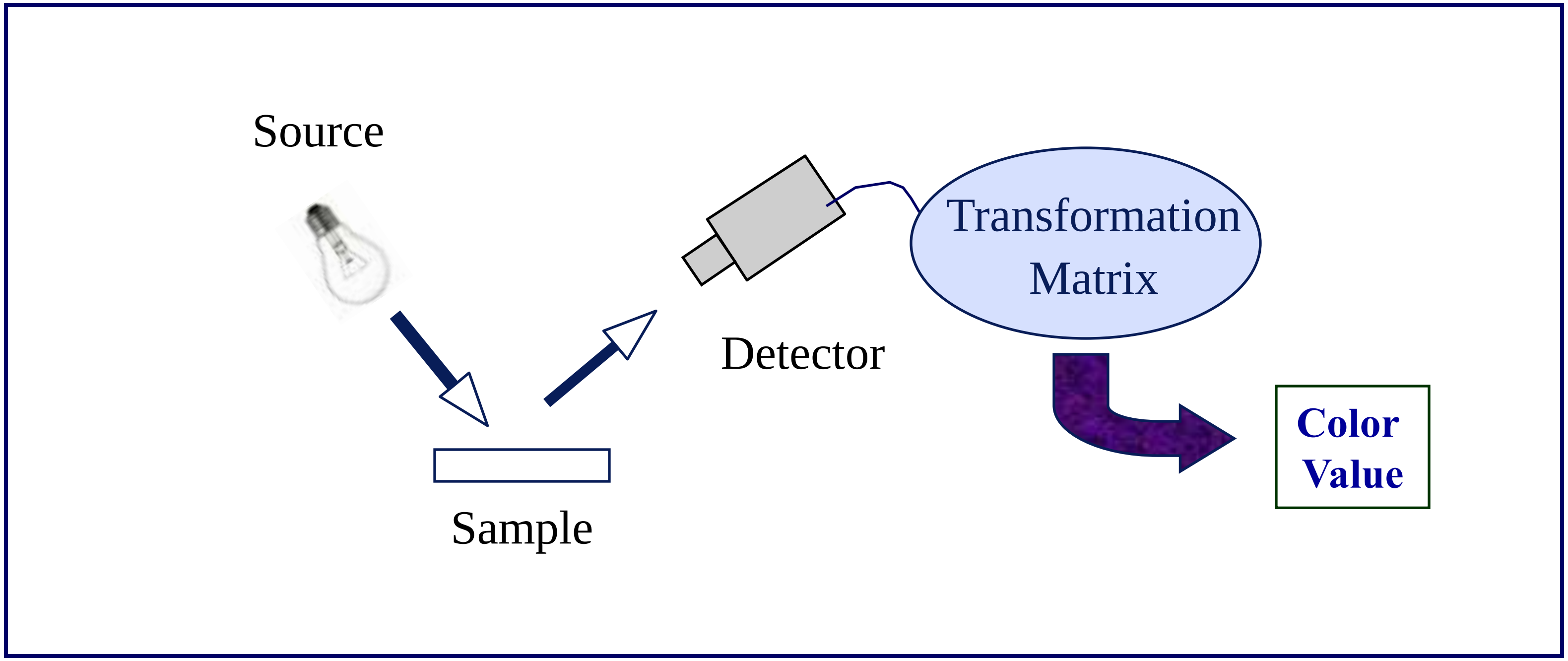
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Outline

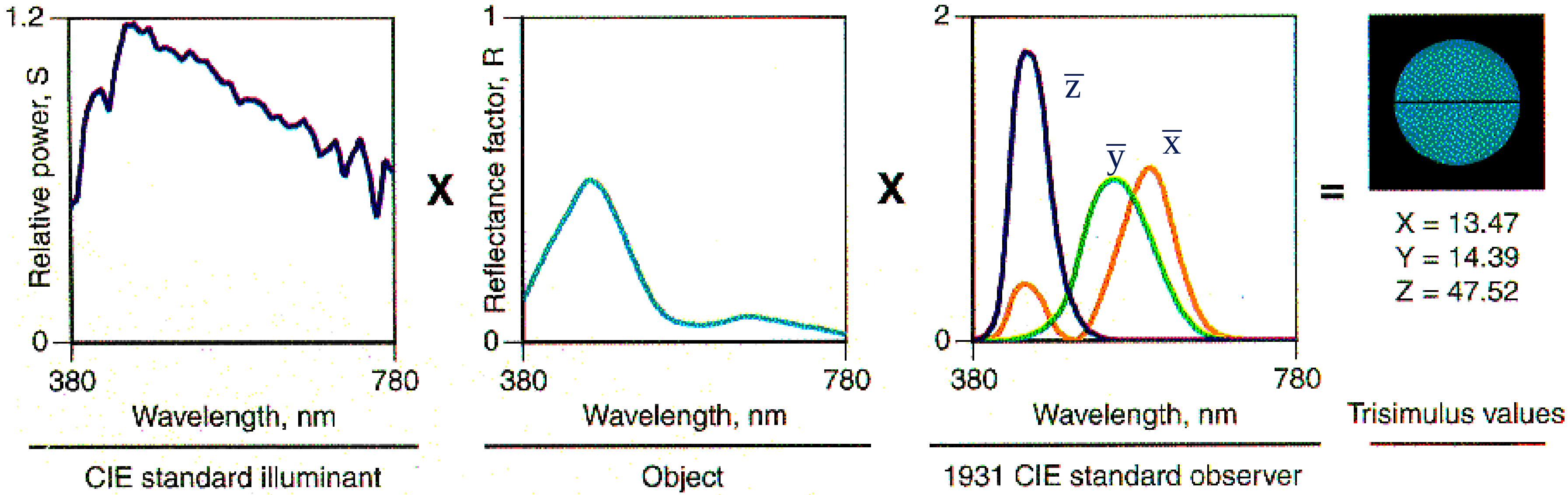
- Basics of Colorimetry
- Color Measuring Instruments and Sources of Uncertaities
- Uncertainties in Reflectance Factor (spectral instruments)
  - Sensitivity Coefficients and Propagation
  - Calculations
  - Results
- Practical Applications
- Conclusions
- References

Colorimetry

is the science used to quantify and describe physically the human perception



CIE (*International Commission on Illumination*) Colorimetric System



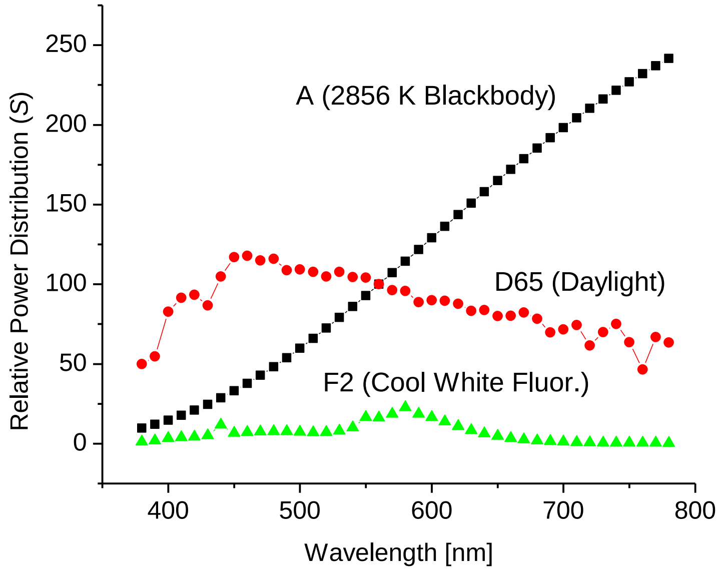
- G. Priest, Phys. Rev. (2) 11, 502 (1918).
- R. Davis and K. S. Gibson, NBS Misc. Pub. No. 114, 21 Jan. 1931.

- D. B. Judd, J. Res. NBS 4, 515 (1930)
- D. B. Judd, J. Opt. Soc. Am. 23, 359 (1933)
- D. B. Judd, J. Opt. Soc. Am. 39, 945 (1949)
- I. Nimeroff, J. Opt. Soc. Am. 54, 696 (1964)

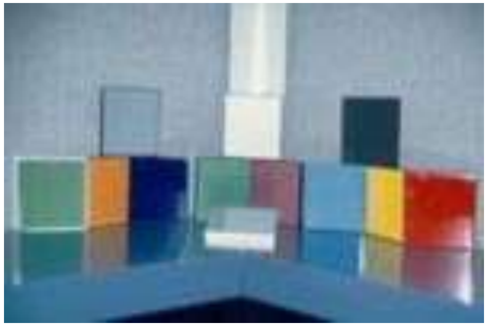
CIE Standard Illuminants

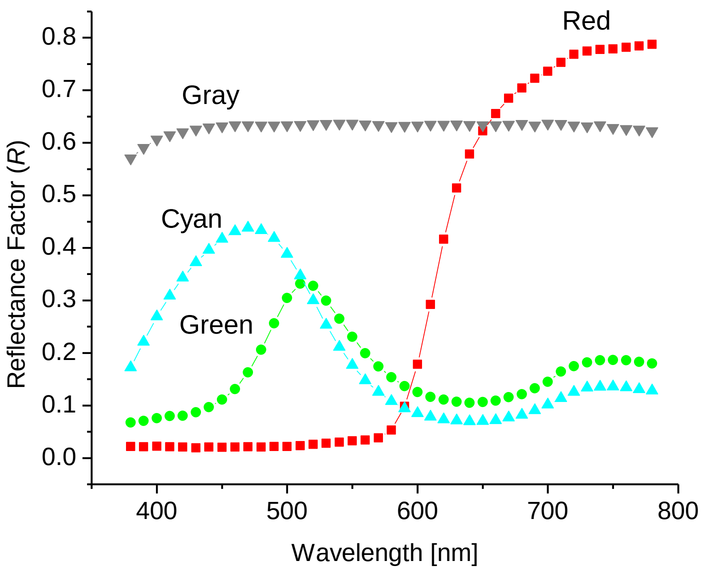
– A Standard Illuminant has a specified spectral power distribution defined by a standardizing organization –

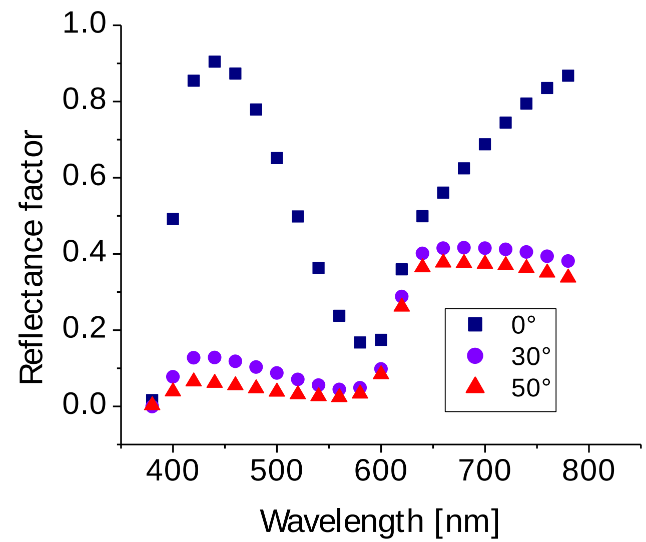
1. Illuminant A (CCT: 2856 K)
   a) Tungsten - filament
2. Daylight Illuminants (CCT: ~6500 K)
   a) D50 (Graphic Arts)
   b) D55 (Photographic applications)
   c) D65 (Paint, textile industries)
3. Fluorescent Lamp Sources
   a) F2 (Cool white; CCT 4200 K)
   b) F7 (Broad-band daylight lamp; CCT 6500 K)
   c) F11 (Narrow-band white; CCT 4000 K)



Spectral Reflectance



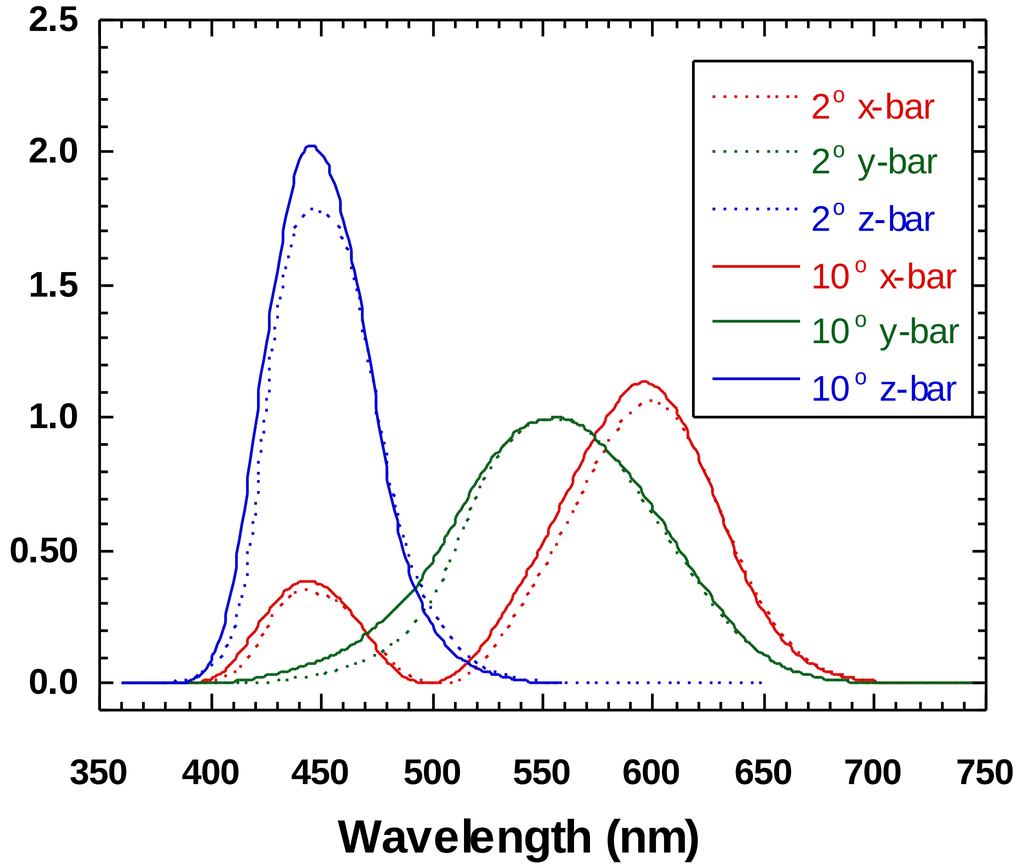




- Only Source of Uncertainty-

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Color Matching Functions: CIE Standard Observers



- Show how the cones in the eye response to light of different wavelength
- Form the basis for the CIE description of color

Tristimulus Values

For object colors

$$X = k\int_{\lambda} S(\lambda)\,R(\lambda)\,\bar{x}(\lambda)\,\mathrm{d}\lambda$$

$$Y = k\int_{\lambda} S(\lambda)\,R(\lambda)\,\bar{y}(\lambda)\,\mathrm{d}\lambda$$

$$Z = k\int_{\lambda} S(\lambda)\,R(\lambda)\,\bar{z}(\lambda)\,\mathrm{d}\lambda$$

$R(\lambda)$: Spectral reflectance factor of object surface.

$S(\lambda)$: Spectral distribution of illumination.

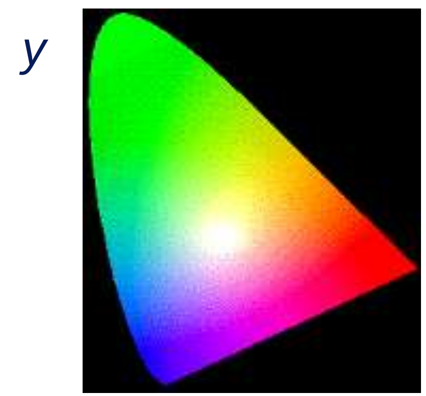
$$k = 100 \Big/ \int_{\lambda} S(\lambda)\,\bar{y}(\lambda)\,\mathrm{d}\lambda$$

Y gives *luminance factor* of the surface in % (for the given illumination).

Chromaticity and Color Space

1. Chromaticity Coordinates *x, y*

$$x = \frac{X}{X+Y+Z} \qquad y = \frac{Y}{X+Y+Z}$$



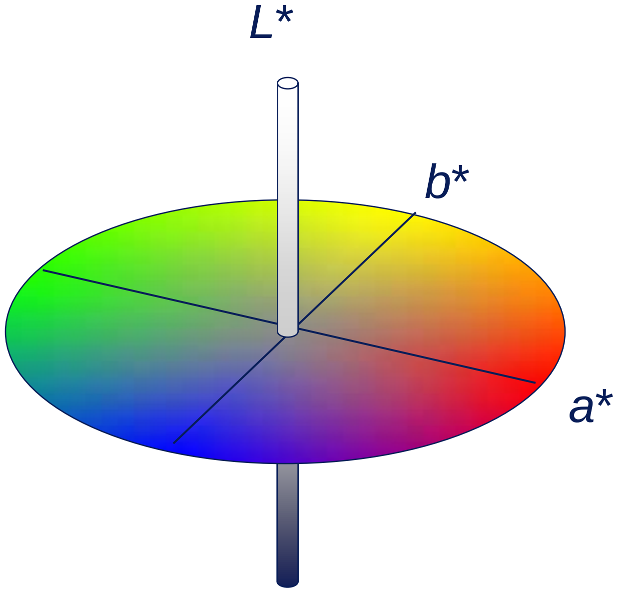
2. Color Space *L*, a*, b**

$$L^* = 116\left(\frac{Y}{Y_n}\right)^{1/3} - 16$$

$$a^* = 500\left[\left(\frac{X}{X_n}\right)^{1/3} - \left(\frac{Y}{Y_n}\right)^{1/3}\right]$$

$$b^* = 200\left[\left(\frac{Y}{Y_n}\right)^{1/3} - \left(\frac{Z}{Z_n}\right)^{1/3}\right]$$

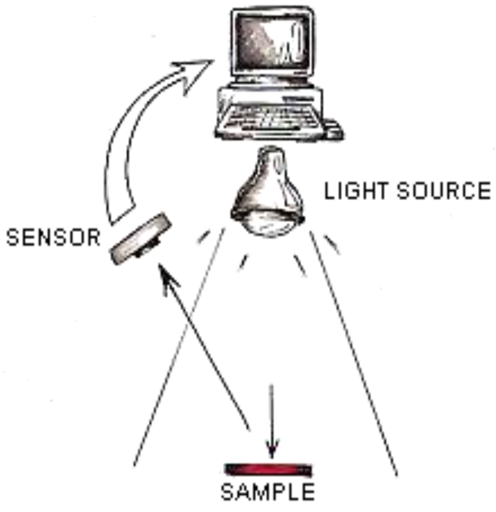
$$\Delta E^*_{ab} = \sqrt{u^2(L^*) + u^2(a^*) + u^2(b^*)}$$



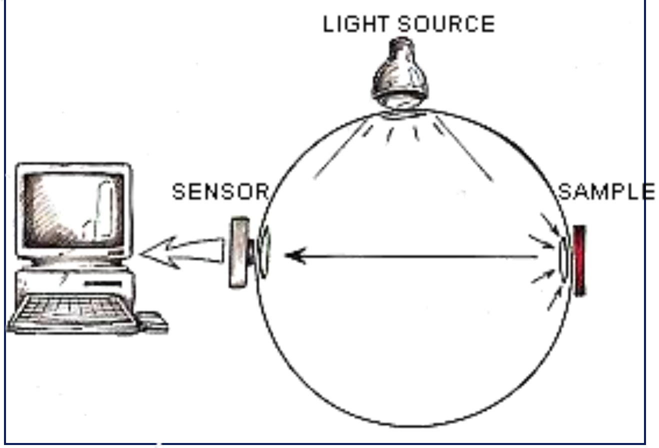
Color Measuring Instruments

Measurement Geometries and Applications

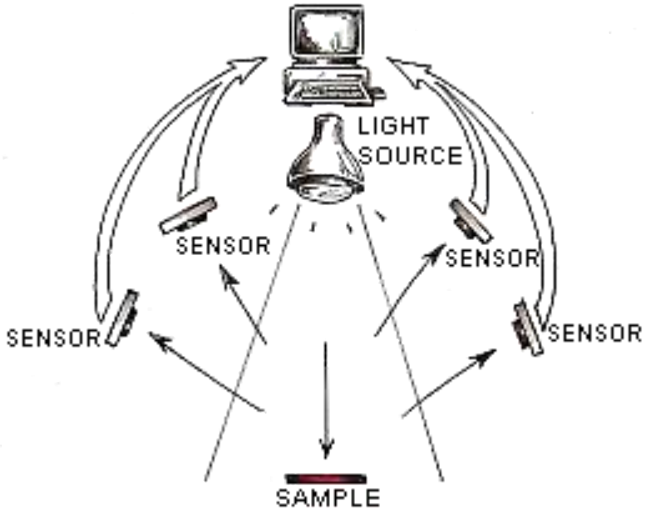
0 /45



Sphere



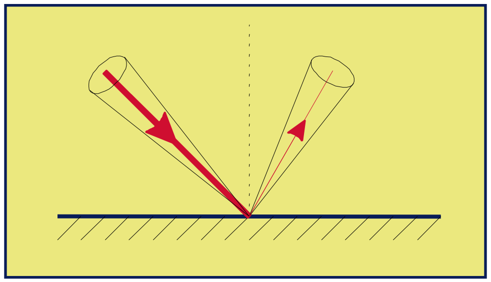
Multi-angle



Practical Geometrical Combinations

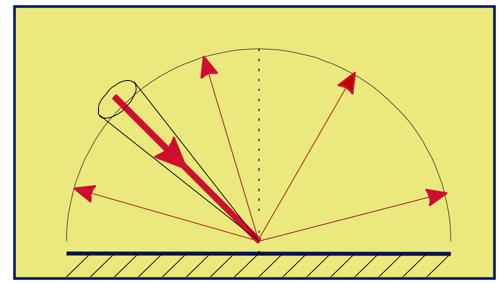
Bi-directional

(specified by 2 cones)



Directional-hemispherical
or
Hemispherical-directional

(specified by 1 cone)

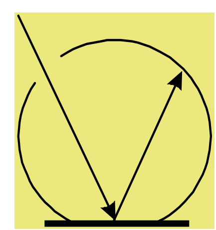


Examples

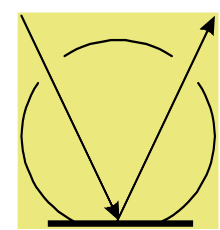
- 0:45 – bi-directional, uniplanar
- 45a:0 – annular illumination, directional viewing
- 0:d – directional-hemispherical
- 8:di – directional-hemispherical, specular component included

specular component

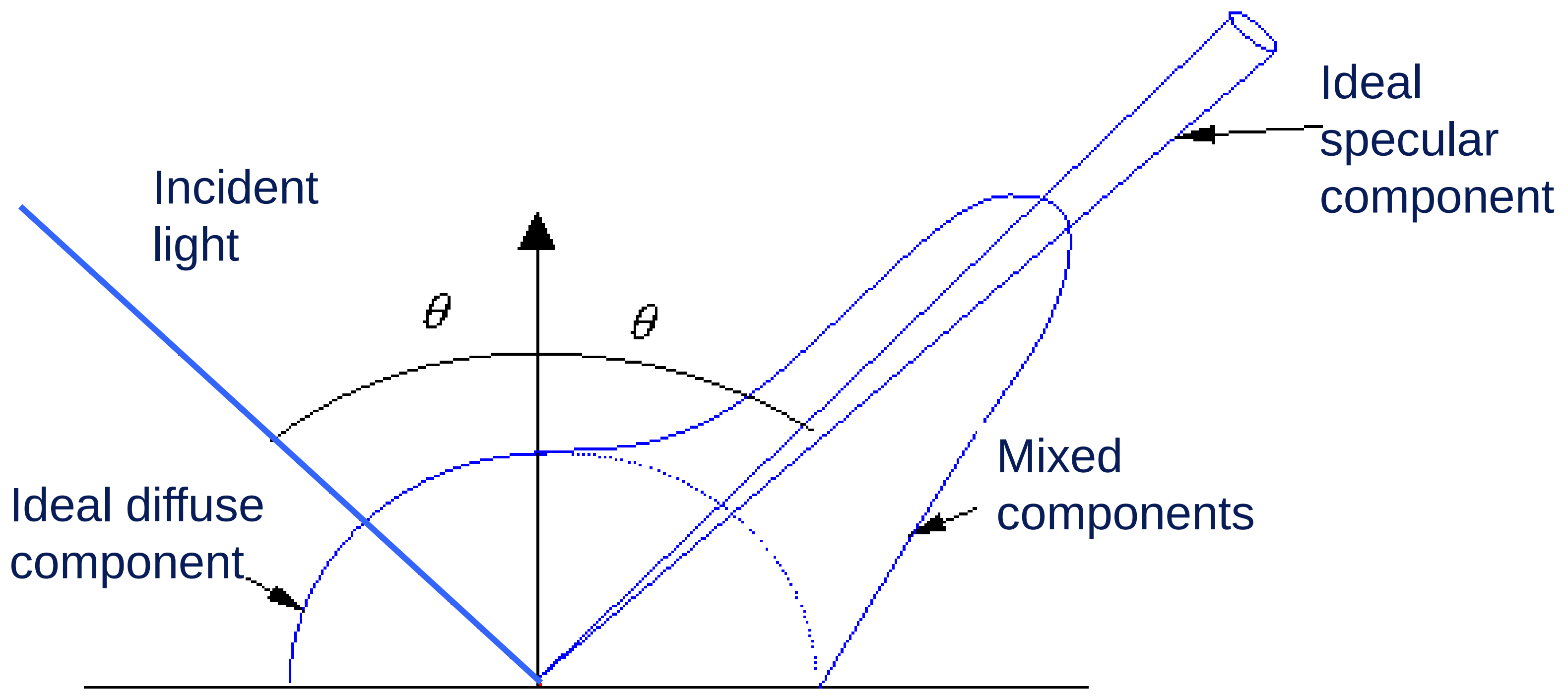
included



excluded



Types of Reflection



For the measurements to have any meaning, we need to specify the wavelength, **direction and solid angle of incident and viewing**, and polarization

Sources of Uncertainty

1. **Light Source**
   a) Stability
   b) Wavelength and bandwidth
   c) Stray-light
2. **Goniometer**
   a) Incident and viewing angles
   b) Mis-alignment of samples
3. **Receiver**
   a) Solid angle – ***absolute measurements***
      i. Area of collection aperture, distance from sample to aperture
   b) Non-linearity, noise, zero offset
   c) Integrating spheres
      i. Gloss properties of standard and sample, Gloss trap error, Specular beam weighting
   d) Tristimulus colorimeters
      i. Filter functions, Spectrum of illuminator
4. **Sample**
   a) Thermochromism and inhomogeneity
   b) Spectral, angular, and polarization dependence
   c) Reflectance factor of transfer standard – ***relative measurement***

*Guide to the Expression of Uncertainty in Measurement, Geneva: International Organization for Standardization

Measurement Equation for Reflectance Factor

1. At each wavelength λ, indexed by subscript i

$$R_{\mathrm{i}} = \frac{S_{\mathrm{i}}}{S_{\mathrm{s,i}}} \cdot R_{\mathrm{s,i}}$$

where
R_{i} – reflectance factor of sample
S_{i} – signal from sample
$S_{\mathrm{s,i}}$ – signal from standard
$R_{\mathrm{s,i}}$ – reflectance factor of standard

- Applies to all geometries (0/45, 0/d, 8/de, etc.)
- Applies to relative and absolute techniques, for absolute, $R_{\mathrm{s}} = \pi/\Omega_{\mathrm{p}}$
- Always a ratio of signals

Uncertainty Analysis

1. Functional relationship

$$y = f(x_1, x_2, \ldots x_i, \ldots x_n)$$

2. Propagation of uncertainty

$$u_c^2(y) = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(\frac{\partial f}{\partial x_i} \right) \left(\frac{\partial f}{\partial x_j} \right) \cdot r(x_i, x_j) \cdot u(x_i) \cdot u(x_j)$$

$\partial f/\partial xi$ – sensitivity coefficient

$u(xi)$ – standard uncertainty of *x*i

$r(x\mathrm{i}, x\mathrm{j})$ – correlation coefficient

$uc(y)$ – combined uncertainty of *y*

Correlations - Ratio

1. Example: $y = a\dfrac{x_1}{x_2}$
2. Sensitivity Coefficients: $\partial y/\partial x_1 = a/x_2$, $\partial y/\partial x_2 = -ax_1/x_2^2$
3. Uncorrelated: $r(x_i, x_j) = 0$; sum-of-squares

$$\frac{u_c^2(y)}{y^2} = \frac{u^2(x_1)}{x_1^2} + \frac{u^2(x_2)}{x_2^2}$$

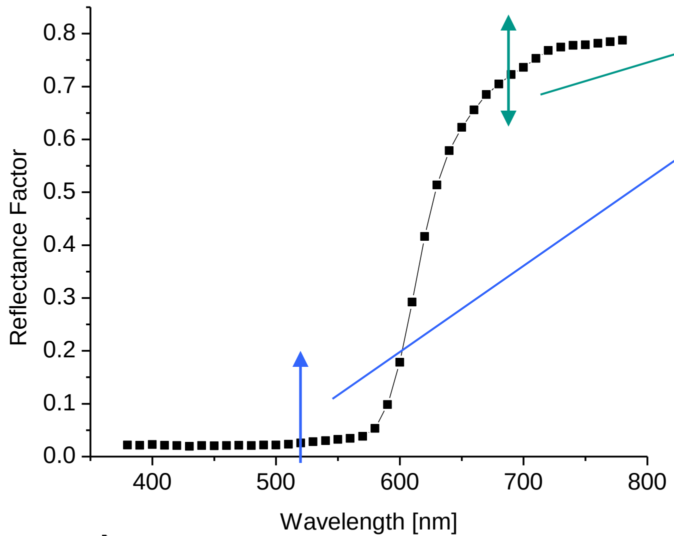
4. Correlated: $r(x_i, x_j) = 1$; square-of-difference

$$\frac{u_c^2(y)}{y^2} = \frac{u^2(x_1)}{x_1^2} + \frac{u^2(x_2)}{x_2^2} - 2\frac{u(x_1)}{x_1}\frac{u(x_2)}{x_2} = \left[\frac{u(x_1)}{x_1} - \frac{u(x_2)}{x_2}\right]^2$$

5. For correlated, if $u(x_1) = u(x_2)$ and $x_1 = x_2$ then $u_c(y) = 0$

Illustration of Uncertainties

1. Y-axis



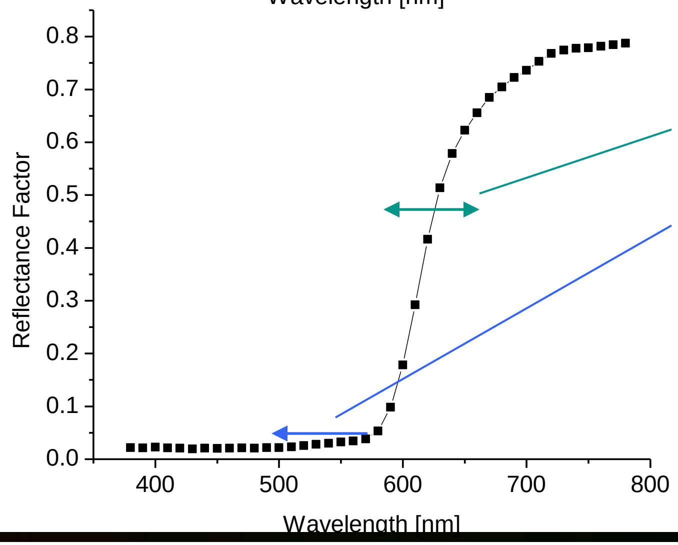
Uncorrelated – Noise

Correlated – Cal. standard

Stray light

Offset

2. X-axis



Uncorrelated – Wavelength

Correlated – Wavelength

Sources of Uncertainty

1. Measurement Equation

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

2. Sources of Uncertainty

a) Signals

Sensitivity coefficients

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

b) Standard

Sensitivity coefficient

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

c) Wavelength

Sensitivity coefficient

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

Uncertainty in Reflectance Factor (1)

1. Propagation of uncertainty

$$u_c^2(y) = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n\text{-}1} \sum_{j=i+1}^{n} \left(\frac{\partial f}{\partial x_i} \right) \left(\frac{\partial f}{\partial x_j} \right) \cdot r(x_i, x_j) \cdot u(x_i) \cdot u(x_j)$$

2. Signals

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

a) Noise

$r(S_i, S_{s,i}) = 0$

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

Uncertainty in Reflectance Factor (2)

1. Signals (cont)
   a) Offset
      i. One signal (e.g. mis-alignment)

$r(S_i, S_{s,i}) = 0$

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

      i. Both signals (e.g. improper zero, stray-light)

$r(S_i, S_{s,i}) = +1$

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

2. Standard

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

3. Wavelength

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

Uncertainties for Green

D65/1964

Noise: $u(S)/S = 0.001$

Offset: $u(S)/S = 0.001$

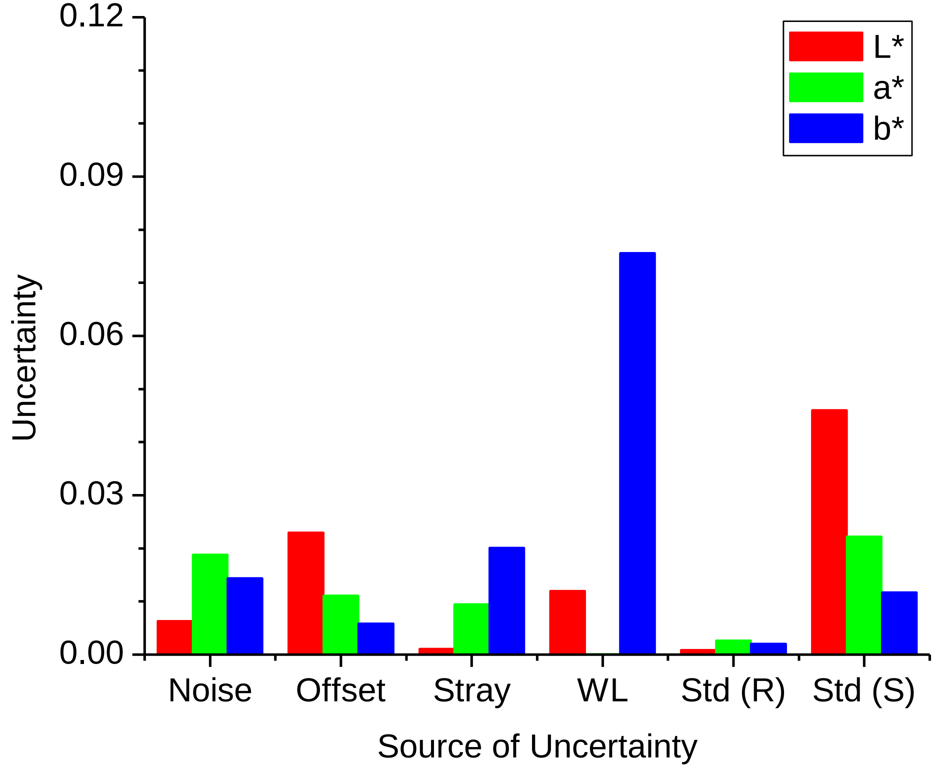
Stray light: 10^{-6} rejection

Wavelength: $u(\lambda) = 0.1$ nm

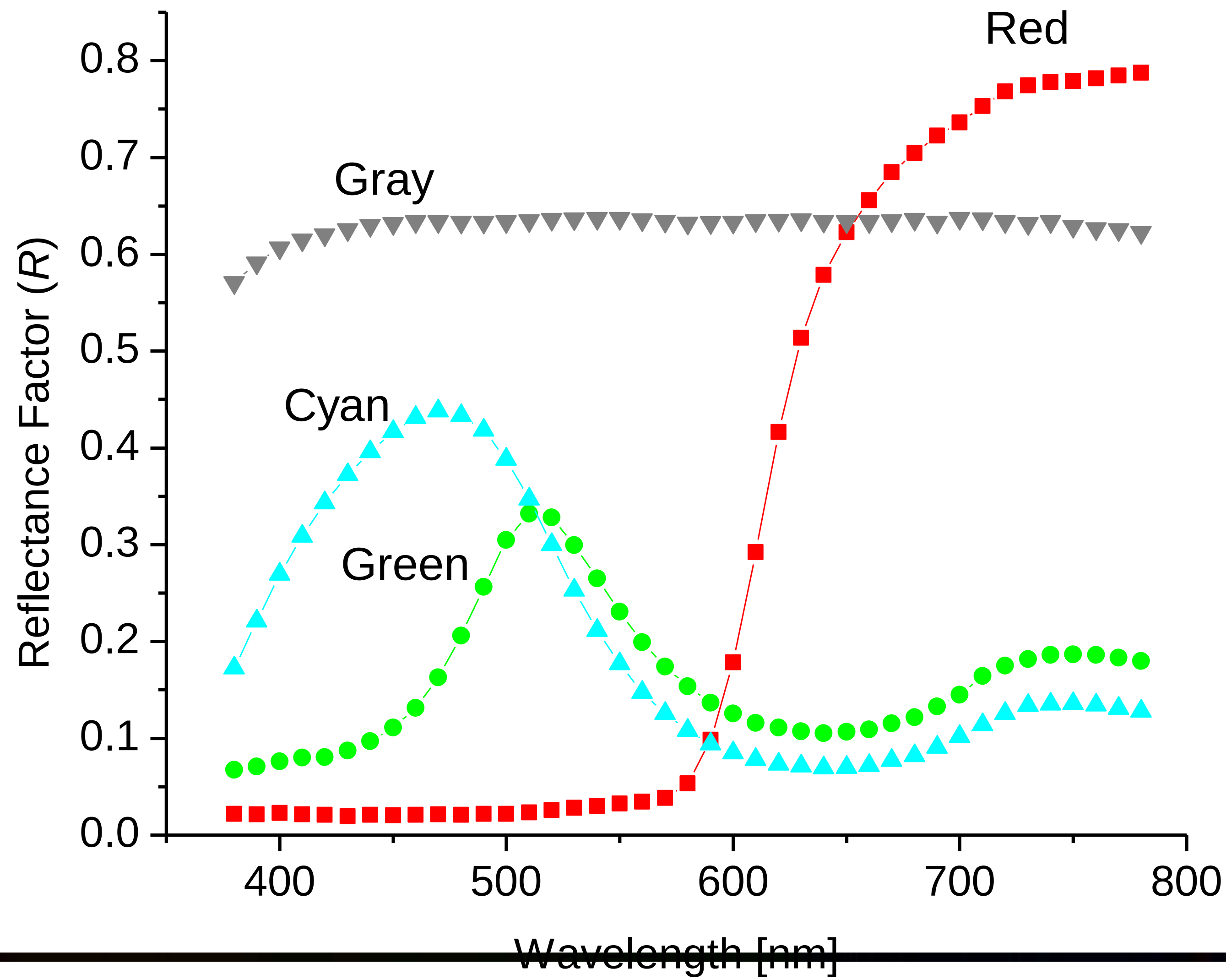
Standard

Random: $u(Rs)/Rs = 0.0002$

Systematic: $u(Rs)/Rs = 0.002$

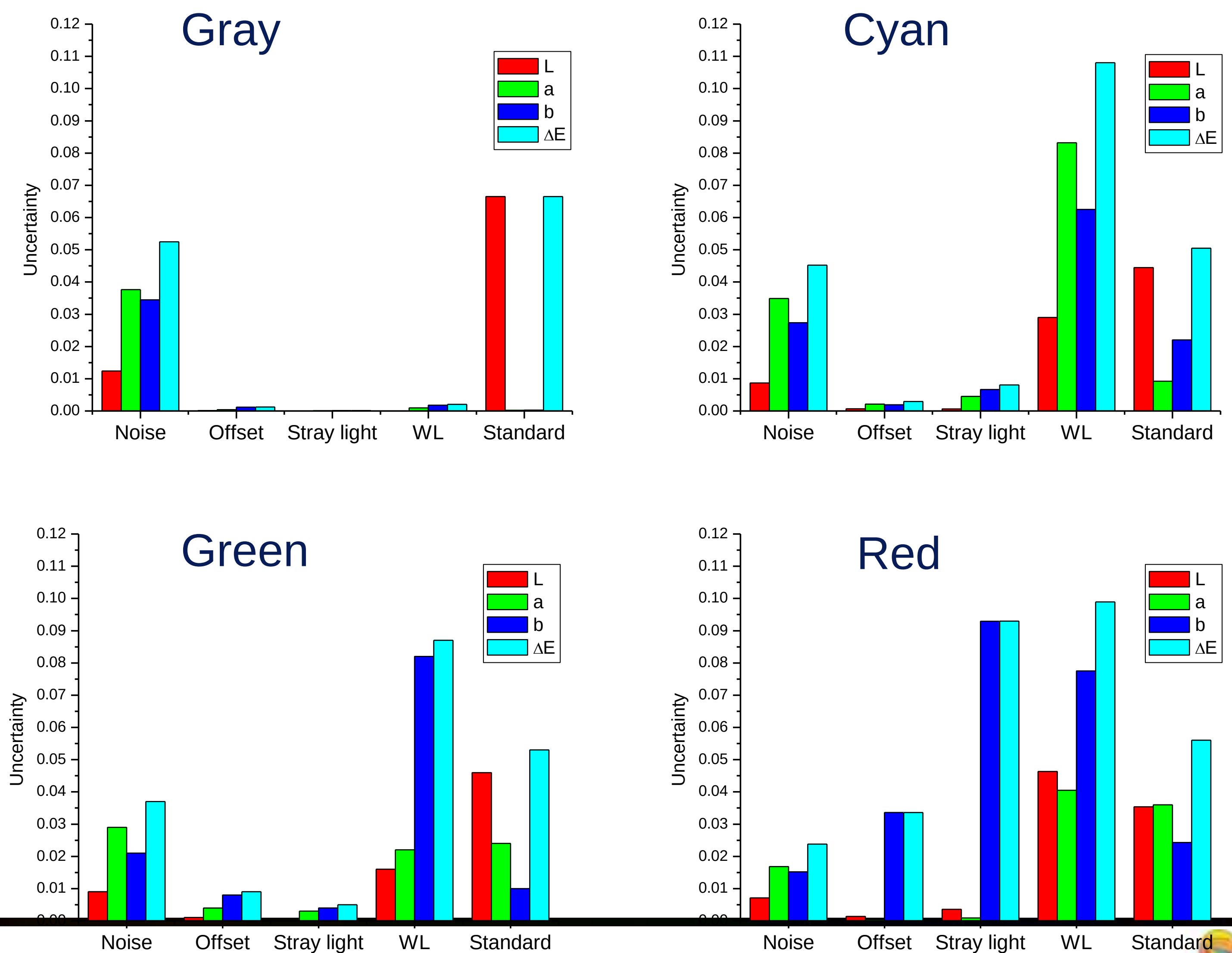


Samples



Red
Gray
Cyan
Green
Reflectance Factor (R)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
400
500
600
700
800
Wavelength [nm]

Uncertainties in *L**, *a**, *b**

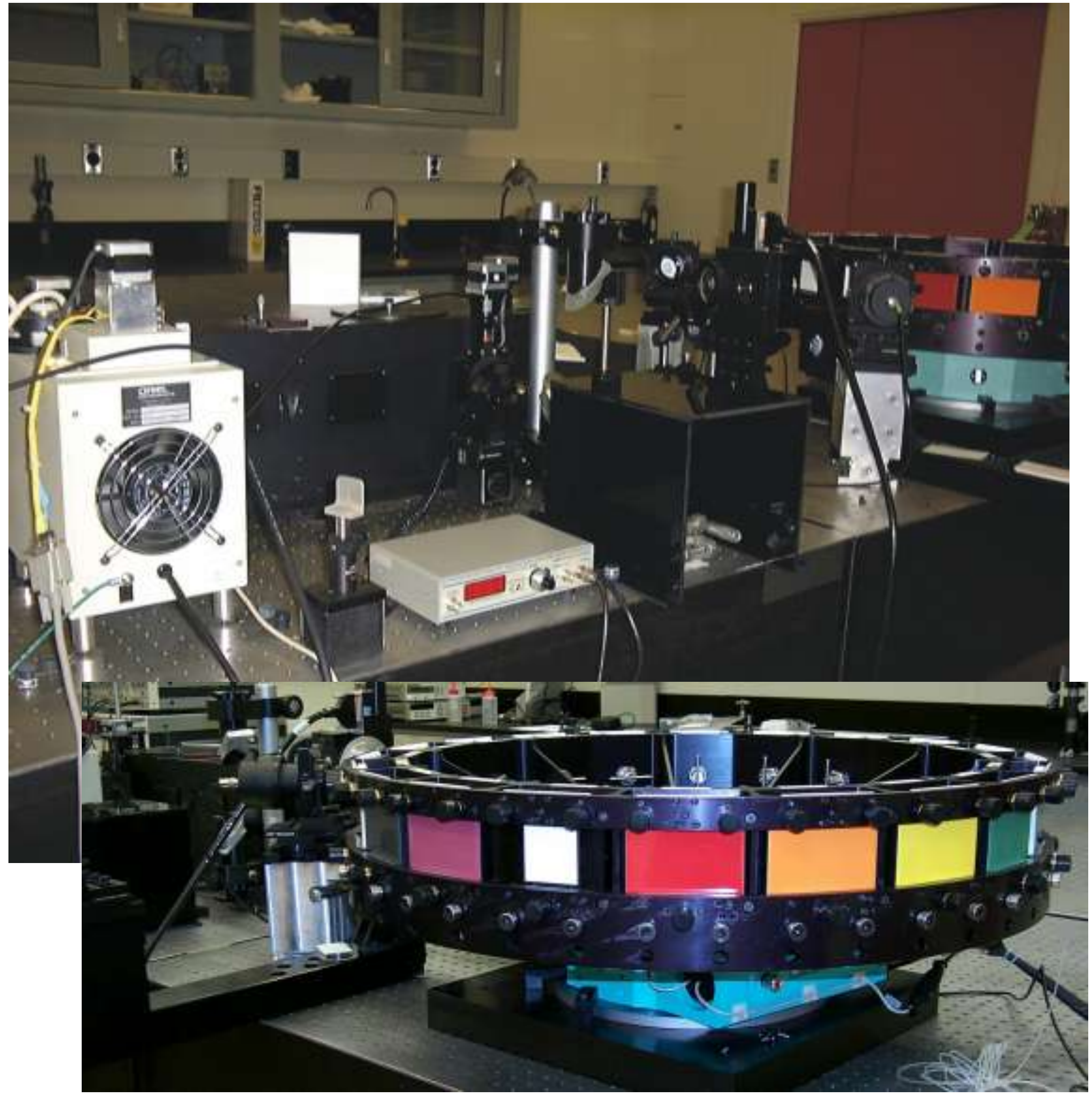


Comparison of Instrument Design

		ΔE^*_{ab}			
Source	**Inst. Type**	**Gray**	**Cyan**	**Green**	**Red**
Noise	Good $\varepsilon = 0.001$	0.053	0.045	0.037	0.024
	Fair $\varepsilon = 0.01$	0.525	0.452	0.374	0.238
Offset	Good $\varepsilon = 0.00001$	0.001	0.003	0.009	0.034
	Fair $\varepsilon = 0.0001$	0.012	0.029	0.090	0.336
Stray light	Good $n = 6$	0.000	0.008	0.005	0.093
	Fair $n = 4$	0.016	0.808	0.477	9.300
Wavelength	Good $u = 0.1$ nm	0.002	0.108	0.087	0.099
	Fair $u = 0.5$ nm	0.010	0.540	0.433	0.495
Standard	Both $u = 0.002$	0.066	0.050	0.053	0.056
Total	***Good***	***0.085***	***0.128***	***0.109***	***0.153***
	Fair	***0.530***	***1.073***	***0.752***	***9.322***

NIST 0 /45 ***Relative*** Reflectance Colorimeter

1. Double grating monochromator: wavelength uncertainty: .05 nm and stray light: 10^{-6}
2. Collimated, monochromatic, polarized beam of light (360 nm to 800 nm)
3. Measurements of 0 /45 spectral reflectance factors for colored, non-fluorescent samples
4. Scale realization - transfer from STARR using Spectralon™ plaques



Uncertainty Budget for 0 /45 Colorimeter

Component of uncertainty	Relative expanded uncertainty (k = 2) [%]				
		White		Green	
		400 nm	800nm	400nm	800nm
Noise		0.17	0.07	0.97	0.23
Wavelength (0.05nm)		0.06	0.00	0.13	0.02
Stray-light (~10^{-6})		0.02	0.00	0.64	0.00
Offset		0.39	0.40	0.40	0.40
Reference Standard (Systematic)		0.39	0.40	0.41	0.41
Reference Standard (Random)		0.03	0.03	0.03	0.03
	Relative combined expanded uncertainties (k = 2) [%] 400 nm				
		0.58		**1.30**	

Compare Measurements to Determine **Color Matching**

- ✓ Two samples on one instrument, e.g. standard and test for process control
  - Limited by the noise (repeatability) of the instrument
  - Traceability is not an issue
- ✓ One sample on two instruments e.g. acceptance of item from a vendor by a customer
- ✓ Two samples on two instruments e.g. two items provided by two vendors to be assembled by a customer
  - Traceability is an issue
  - Instrument maker, model, …
  - **Calibration Standard**

Parameters to Consider

1. Sample
   a) Physical properties (e.g. size, uniformity)
   b) Optical properties (e.g. color, appearance)
2. Instrument
   a) Geometry (bidirectional 0:45, 0:45c, 0:45a, etc. or hemispherical 0:d, 8:di, 8:de, etc.)
   b) Manufacturer
   c) Model
   d) Serial Number
3. Traceability
   a) Standard
   b) Vendor
   c) National Metrology Institute (NMI)

Traceability Chain - unbroken chain of comparisons, all having stated uncertainties

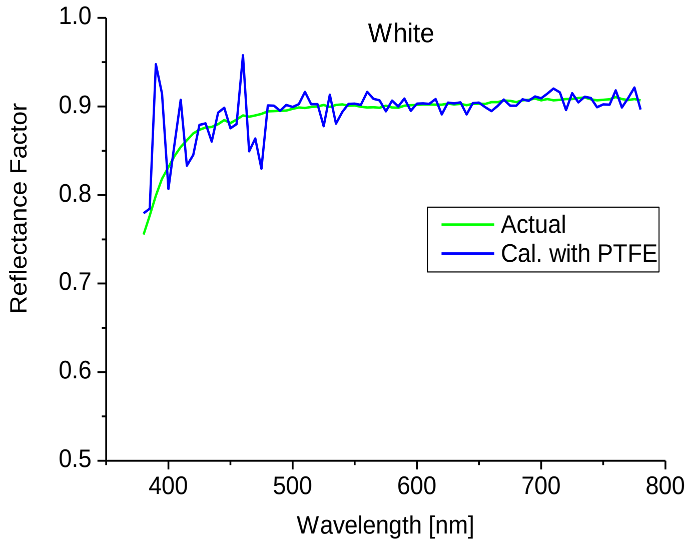
Group	Instrument	Standard	Example
NMI	NMI Reference		
NMI		Reference	White Standard
NMI	NMI Transfer		
NMI / Manuf.		Primary	Color tiles
Manuf.	Manuf. Reference		
Manuf.		Secondary	Paint Set
Manuf.	Manuf. Model		
Manuf. / Customer		Instrument	Paint Set
Customer	Manuf. S/N		
Customer		Test	Paint

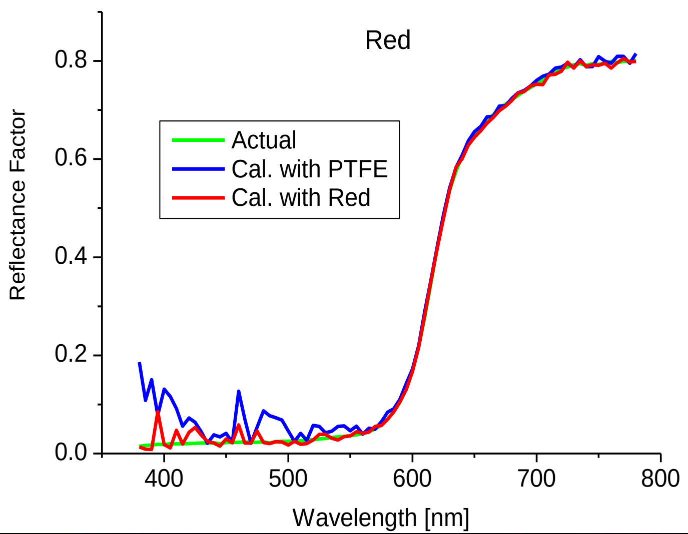
Increasing Uncertainty ↓

The more two chains have in common, the lower the uncertainty of the comparison

Uncertainty from Noise

1. Description
    a) Random effect on all signals
    b) No correlations
    c) Modeled as a fixed fraction of the maximum signal
2. Effect for D65/10° with fraction = 1 %

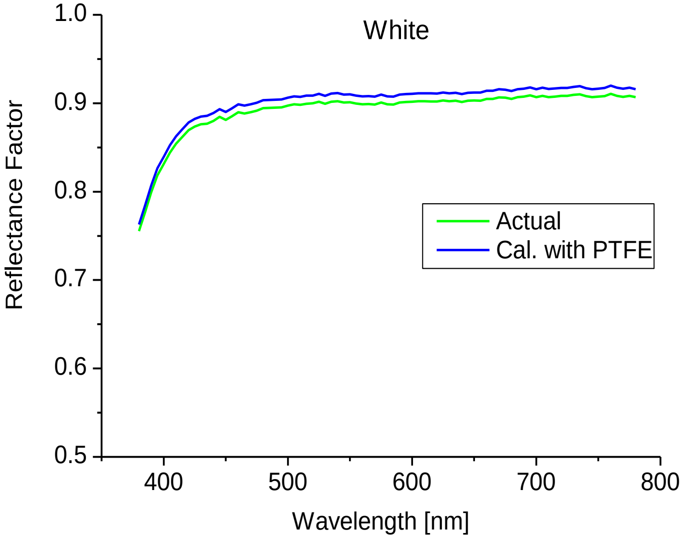




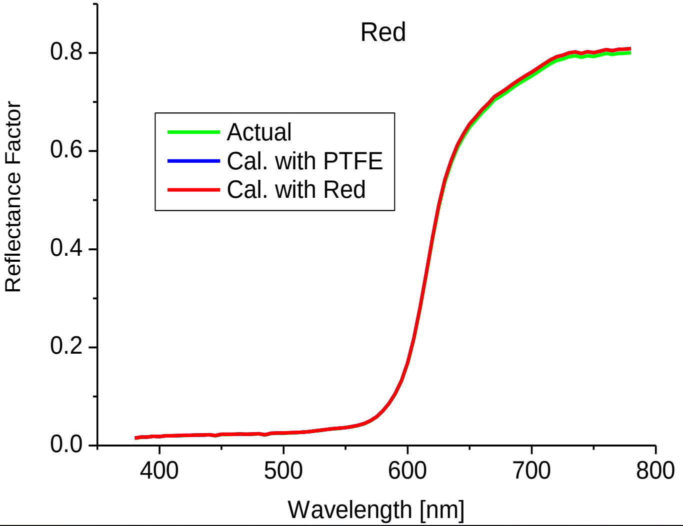
Sample	White	Red	
Standard	PTFE	PTFE	Red
u(*L**)	0.512	0.524	0.349
u(*a**)	1.446	1.524	1.125
u(*b**)	1.236	5.373	3.890

Uncertainty from Offset

1. Description
   a) Systematic effect on sample signals, for example, from mis-alignment
   b) Correlated
   c) Modeled as a fixed fraction of the signal
2. Effect for D65/10° with fraction = 1 %



Sample	White	Red	
Standard	PTFE	PTFE	Red
u(*L**)	0.373	0.177	0.169
u(*a**)	0.001	0.163	0.125
u(*b**)	0.004	0.118	0.098

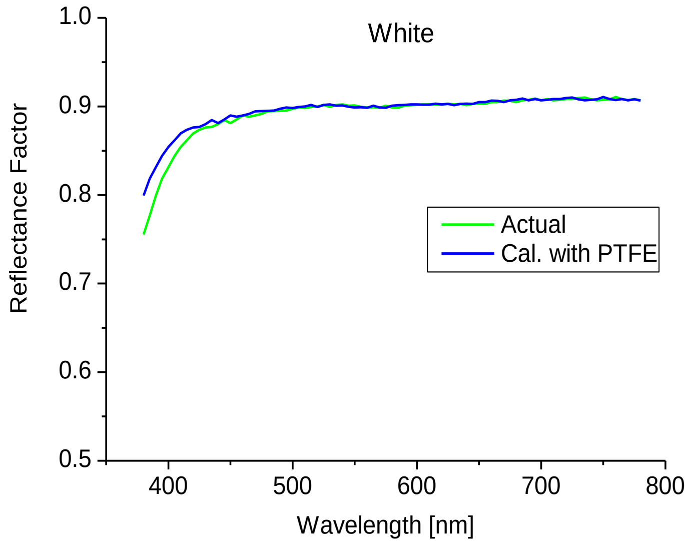


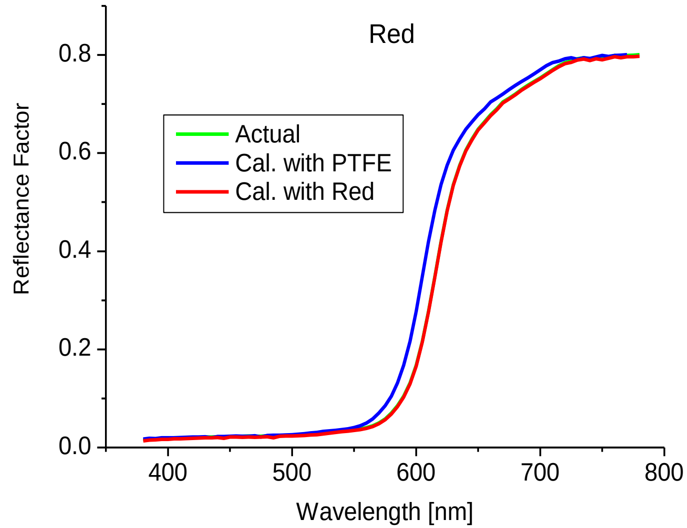
Uncertainty from Wavelength

1. Description
   a) Systematic effect on all signals from instrument wavelength calibration
   b) Correlated
   c) Modeled as $$u(S) = \frac{\partial \left(S / S_s \right)}{\partial \lambda} \cdot u(\lambda)$$

2. Effect for D65/10° with $u(\lambda)$ = 10 nm

Sample	White	Red	
Standard	PTFE	PTFE	Red
u(*L**)	0.010	4.433	0
u(*a**)	0.065	4.707	0
u(*b**)	0.310	7.234	0





Propagating Uncertainties

1. Uncertainty in Reference Standard – PTFE
   a) Sources are noise, geometry (distances and angles), linearity of detector, wavelength of monochromator, reflectance properties of PTFE
   b) Uncertainty in Rs is 0.2 % for both bi-directional (e.g. 0:45) and directional-hemispherical (e.g. 8:di) geometries
2. Use $\Delta E = \sqrt{u^2(L^*) + u^2(a^*) + u^2(b^*)}$ as a measure of uncertainty
3. Consider propagation of uncertainty through traceability chain for white and red samples for D65/10°
   a) Measure white test sample using traceability chain based on white standards
   b) Measure red test sample using traceability chain based on white standards
   c) Measure ret test sample using traceability chain based on red standards

Uncertainties in Standards and Test Sample

Standard Type	Standard	ΔE	Standard	ΔE	Standard	ΔE
Reference	PTFE		PTFE		PTFE	
Primary	White	0.11	White	0.11	Red	0.18
Secondary	White	0.14	White	0.14	Red	0.20
Instrument	White	0.28	White	0.28	Red	0.31
Test	White	0.30	Red	14.34	Red	0.42

Notes: Large uncertainty for red test sample using instrument calibrated with white standard due to stray-light

Noise is the only uncertainty contribution for test samples using instrument calibrated with a standard of the same color

Summary

1. Consider typical sources of uncertainty – noise, offset, dark, stray-light, wavelength, standard
2. Assign standard uncertainties *u* to these sources
3. Calculate $u(R_i)$ for each source, using the measurement equation and taking correlations between signals into account with $r(S_i, S_{s,i})$
4. In general, colors with large, abrupt changes in reflectance factor have the greatest uncertainty in the calculated values
5. Whenever possible, calibrate an instrument using a standard that is similar to the sample to reduce correlated uncertainties in the signals and uncertainty due to wavelength
6. Evaluate the traceability chains to obtain the uncertainty for a comparison between two instruments
   a) The more the two chains have in common, the lower the uncertainty of the comparison

References

1. Berns and Petersen, "Empirical Modeling of Systematic Spectrophotometric Errors," Color Res. Appl. 13, 243 (1988)
2. Fairchild and Reniff, "Propagation of Random Errors in Spectrophotometric Colorimetry," Color Res. Appl. 16, 361 (1991)

- G. Wyszecki and W. S. Stiles, "Color Science: Concepts and Methods, Quantitative Data and Formulae," John Wiley and Sons, New York, 1982.
- M. E. Nadal, E. A. Early, and R. R. Bousquet "NIST Measurement Services: 0:45 Surface Color," NIST Spec. Pub. 250-71, U. S. Dept. of Commerce (2008).
- M. E. Nadal, E. A. Early, W. Weber, and R. Bousquet, "NIST 0:45 Reflectometer," *Color Res. Appl*, 33, 94-99 (2008).
- E. A. Early and M. E. Nadal, "Uncertainty Analysis for the NIST 0:45 Reflectometer," *Color Res. Appl.*, 33, 100-107 (2008).