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UNCERTAINTY ANALYSIS FOR DIFFUSE REFLECTANCE OF A GOLD SAMPLE AS DERIVED FROM NIST VALUES OF PTFE REFLECTANCE

Calculating uncertainty in measurements is something that is increasingly required nowadays. It is also one of those things that you either know how to do or you don't. Descriptions and literature tend to be mathematical, and quick and easy teaching guides are rare.

To help our customers, Optronic Laboratories has created an example spreadsheet. It is for a diffuse reflectance measurement of a gold sample using Optronic Laboratories's equipment but contains many of the elements you might need for other measurements. That is the first key to understanding uncertainties; that uncertainties apply to measurements and hence depend on samples, conditions and equipment. Other keys are found throughout this spreadsheet in the form of procedures, formulas and comments.

This document provides some of the justifications to the spreadsheet for those customers who can follow the math. Basically, to show how uncertainties in components relate to the result, we start with the measurement equation. Using Optronic Laboratories's' OL750 Series measurement systems

$$\rho_\lambda^T = \frac{s4_\lambda}{s3_\lambda} \cdot \frac{s1_\lambda}{s2_\lambda} \rho_\lambda^S$$

configured for diffuse reflectance, four scans [s1 through s4] are made *(as detailed in the spreadsheet)*. The reflectivity of a sample under test, $\rho^T\lambda$, is related to the reflectivity of a

$$u^2(\rho_\lambda^T) = \left(\frac{d\rho_\lambda^T}{ds1_\lambda}\right)^2 u^2(s1_\lambda) + \left(\frac{d\rho_\lambda^T}{ds2_\lambda}\right)^2 u^2(s2_\lambda) + \left(\frac{d\rho_\lambda^T}{ds3_\lambda}\right)^2 u^2(s3_\lambda) + \left(\frac{d\rho_\lambda^T}{ds4_\lambda}\right)^2 u^2(s4_\lambda) + \left(\frac{d\rho_\lambda^T}{d\rho_\lambda^S}\right)^2 u^2(\lambda_\lambda^S)$$

standard, $\rho^S{}_\lambda$, by:

$$\frac{d\rho_\lambda^T}{ds1_\lambda} = \frac{s4_\lambda \cdot \rho_\lambda^S}{s3_\lambda \cdot s2_\lambda} \quad , \frac{d\rho_\lambda^T}{ds2_\lambda} = \frac{-s4_\lambda \cdot s1_\lambda \cdot \rho_\lambda^S}{s3_\lambda \cdot s2_\lambda^2} \quad , \frac{d\rho_\lambda^T}{ds3_\lambda} = \frac{-s4_\lambda \cdot s1_\lambda \cdot \rho_\lambda^S}{s3_\lambda^2 \cdot s2} \quad , \frac{d\rho_\lambda^T}{ds4_\lambda} = \frac{s4_\lambda \cdot \rho_\lambda^S}{s3_\lambda \cdot s2_\lambda} \quad , \frac{d\rho_\lambda^T}{d\rho_\lambda^S} = \frac{s4_\lambda \cdot s1_\lambda}{s3_\lambda \cdot s2_\lambda}$$

The variance in $\rho\lambda^T$ (variance is the square of the uncertainty) is related to the variances in the signals and the sensitivity of $\rho\lambda^T$ to the signals. Mathematically, assuming no correlation:

Differentiating the measurement equation gives us the sensitivity components:

Hence, the relative variance is then given by:

$$\frac{u^2(\rho_\lambda^T)}{(\rho_\lambda^T)^2} = \frac{\left(\frac{s4_\lambda^2 \cdot (\rho_\lambda^S)^2 \cdot u^2(s1_\lambda)}{s3_\lambda^2 \cdot s2_\lambda^2}\right)}{\left(\frac{s4_\lambda^2}{s3_\lambda^2} \cdot \frac{s1_\lambda^2}{s2_\lambda^2} \cdot (\rho_\lambda^S)^2\right)} + \frac{\left(\frac{s4_\lambda^2 \cdot s1_\lambda^2 \cdot (\rho_\lambda^S)^2 \cdot u^2(s2_\lambda)}{s3_\lambda^2 \cdot s2_\lambda^4}\right)}{\left(\frac{s4_\lambda^2}{s3_\lambda^2} \cdot \frac{s1_\lambda^2}{s2_\lambda^2} \cdot (\rho_\lambda^S)^2\right)} + \frac{\left(\frac{s4_\lambda^2 \cdot s1_\lambda^2 \cdot (\rho_\lambda^S)^2 \cdot u^2(s3_\lambda)}{s3_\lambda^4 \cdot s2_\lambda^2}\right)}{\left(\frac{s4_\lambda^2}{s3_\lambda^2} \cdot \frac{s1_\lambda^2}{s2_\lambda^2} \cdot (\rho_\lambda^S)^2\right)}$$

$$+ \frac{\left(\frac{s4_\lambda^2 \cdot (\rho_\lambda^S)^2 \cdot u^2(s4_\lambda)}{s3_\lambda^2 \cdot s2_\lambda^2}\right)}{\left(\frac{s4_\lambda^2}{s3_\lambda^2} \cdot \frac{s1_\lambda^2}{s2_\lambda^2} \cdot (\rho_\lambda^S)^2\right)} + \frac{\left(\frac{s4_\lambda^2 \cdot s1_\lambda^2 \cdot u^2(\rho_\lambda^S)}{s3_\lambda^2 \cdot s2_\lambda^2}\right)}{\left(\frac{s4_\lambda^2}{s3_\lambda^2} \cdot \frac{s1_\lambda^2}{s2_\lambda^2} \cdot (\rho_\lambda^S)^2\right)}$$

$$= \frac{u^2(s1_\lambda)}{s1_\lambda^2} + \frac{u^2(s2_\lambda)}{s2_\lambda^2} + \frac{u^2(s3_\lambda)}{s3_\lambda^2} + \frac{u^2(s4_\lambda)}{s4_\lambda^2} + \frac{u^2(\rho_\lambda^S)}{(\rho_\lambda^S)^2}$$

The relative uncertainty in $\rho\lambda^T$ is therefore related to the relative uncertainties in the signals and the standard by:

Table 1. Uncertainty Budget for measurements at 900nm.

$$\frac{u(\rho_\lambda^T)}{\rho_\lambda^T}=\sqrt{\left(\frac{u(s1_\lambda)}{s1_\lambda}\right)^2+\left(\frac{u(s2_\lambda)}{s2_\lambda}\right)^2+\left(\frac{u(s3_\lambda)}{s3_\lambda}\right)^2+\left(\frac{u(s4_\lambda)}{s4_\lambda}\right)^2+\left(\frac{u(\rho_\lambda^S)}{\rho_\lambda^S}\right)^2}$$

COMPONENT	UNCERTAINTY IN COMPONENT	DISTRIBUTION	EVALUATION TYPE	DEGREES OF FREEDOM	SENSITIVITY	UNCERTAINTY CONTRIBUTION
SPECTRAL IRRADIANCE						
PTFE Standard Values	0.050%	Rectangular	B	Infinite	1	0.050%
Scan 1	0.023%		A	10	1	0.023%
Scan 2	0.020%		A	5	1	0.020%
Scan 3	0.016%		A	5	1	0.016%
Scan 4	0.009%		A	5	1	0.009%
Amplifier Linearity	0.100%	Rectangular	B	Infinite	1	0.100%
System Drift	0.045%	Rectangular	A	Infinite	1	0.045%
Combined Relative Uncertainty in Reflectance [Quadrature Sum]						0.13%
Expanded Relative Uncertainty in Reflectance [k=2]						0.25%
Reflectance Value	96.09%	Uncertainty in Reflectance Value [k=2]			0.24%	

The uncertainty value is expressed at k=2, which corresponds to approximately 95% confidence interval.

$$u^2(\rho_\lambda^T)=\left(\frac{s4_\lambda\cdot\rho_\lambda^S}{s3_\lambda\cdot s2_\lambda}\right)^2u^2(s1_\lambda)+\left(\frac{-s4_\lambda\cdot s1_\lambda\cdot\rho_\lambda^S}{s3_\lambda\cdot s2_\lambda^2}\right)^2u^2(s2_\lambda)+\left(\frac{-s4_\lambda\cdot s1_\lambda\cdot\rho_\lambda^S}{s3_\lambda^2\cdot s2}\right)^2u^2(s3_\lambda)$$
$$+\left(\frac{s4_\lambda\cdot\rho_\lambda^S}{s3_\lambda\cdot s2_\lambda}\right)^2u^2(s4_\lambda)+\left(\frac{s4_\lambda\cdot s1_\lambda}{s3_\lambda\cdot s2_\lambda}\right)^2u^2(\rho_\lambda^S)$$

[i] Amplifier linearity affects ratios when signals differ from one another. Here the signal difference is small and the uncertainty represents the maximum possible uncertainty for this amplifier.

[ii] System drift is determined by measurement. A uniform distribution (all values are equally likely) is assumed.