Application Note No. 01

Methods for single beam substitution error correction for Integrating Sphere Reflectance Spectroscopy Accessories

Quantitation of Single Beam Substitution Correction in Reflectance Spectroscopy Accessories

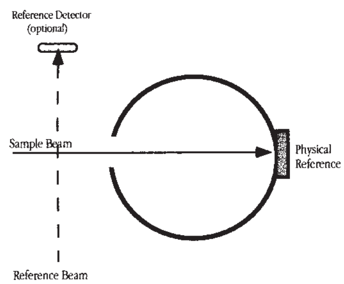

Figure 1. Reference Scan

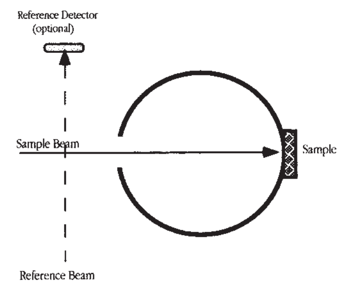

Figure 2. Sample Scan (Sample is substituted for Reference)

The single beam substitution correction, sometimes known as single beam substitution error, is the systematic, predictable, and non-random error inherent in single beam integrating spheres measuring reflectance or transmittance. The error is caused by the difference in the throughput of the sphere when the reference makes up a portion of the sphere wall and when the sample is substituted for the reference (see Figures 1 and 2). In reflectance measurements the throughput and corresponding measured reflectance is usually lower when the sample is present since a reference material of high reflectance (nearly 100%) is used. In transmittance measurements the throughput and the measured transmittance is usually higher when the sample is present since an open port (which has zero reflectance when viewed from inside the sphere) is typically used as a reference.

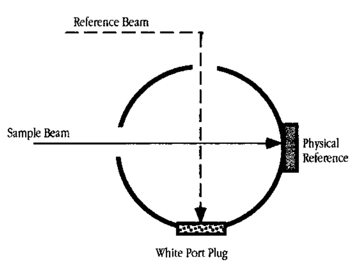

Figure 3. Reference Scan

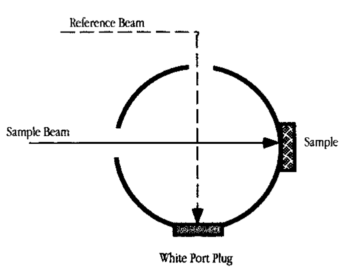

Figure 4. Sample Scan

With spectrophotometers that use a chopped signal between sample and reference this error does not occur. In double beam sphere accessories, the sample and reference beam each 'see' the same sphere. There is an active comparison between throughput with both sample and reference in place, thus there is no substitution error (see Figures 3 and 4).

When a sample and a reference are of similar reflectance, the substitution correction is very small; at worst it may reach as much as 4-5%. In quality control applications where a threshold value is used, this may not be a concern, as the error can simply be built into the threshold. This is also true if only peak position information is required, as single beam correction only concerns the photometric scale.

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Solutions to Substitution Error

There are both physical and mathematical solutions to the problem of single beam substitution error. If the sphere is made sufficiently large and the area of the sample is minimized, the error increasingly diminishes. The use of a large sphere is usually not practical in low cost spectrophotometer systems due to signal-to-noise concerns as well as price considerations.

Use of "Dummy Ports"

In diode array based instruments and in certain dual beam instruments, the sample compartments are usually of sufficient size to allow for a so-called 'dummy port.'

In this geometry, single beam spheres can be designed with an additional comparison port, called a dummy port. The background correction is performed with the physical reference in the sample port and the sample in the dummy port. A second scan is then run with the sample and reference exchanged (see Figures 5 and 6). In the comparison method, the average reflectance and throughput of the sphere remain unchanged from the reference to the sample scan. This technique requires that a separate reference scan be run for each sample scan unless the samples are all almost identical. In this case, the residual substitution error caused by sample-to-sample variation is so small it is negligible.

Mathematical Solution

The mathematical solution is simple in theory, but complex in practice. If a reference is used that is very close in reflectance to the reflectance of the sample, the substitution error becomes negligible. If the user can 'match' the reference reflectance to the reflectance of the sample, or has a large database of different level photometric reflectance standards, one can set up 'look-up' or correction tables to correct for the substitution error. The problem is that such references for all levels of photometric scale are not readily available to users. This article provides such a look-up table for a number of commonly used integrating sphere reflectance accessories.

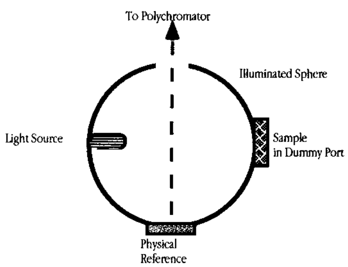

Figure 5. Reference Scan

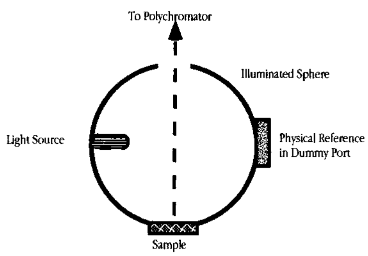

Figure 6. Sample Scan

Twelve Step Single Beam Substitution Error Correction Tables

Tables 1 and 2 show the values for twelve levels of photometric gray scale. The italicized values are the actual reflectance of samples of Labsphere SRS-XX gray scale reflectance material. The values were determined by measuring the corrected 8°/ hemispherical reflectance factor on Labsphere's reference spectrophotometer equipped with a double beam integrating sphere. Similar equipment and techniques are used for measurements of standards at the National Institute of Standards and Technology (NIST), the National Physical Laboratory (NPL) and the National Research Council Canada (NRCC). The second set of values were measured on a dual beam, beam splitter-based spectrophotometer equipped with a Labsphere Single Beam Integrating Sphere Accessory. Because of the sphere size (55 mm i.d.) and measurement geometry of this system, these values also apply to most Labsphere 55 mm single beam sphere accessories.

Using the Twelve Step Single Beam Substitution Error Correction Tables

To use the tables, look at the wavelength of interest, find the corresponding value in the column marked **S** and compare it with the column marked **D** immediately to its left. This is the actual value of reflectance of the sample at that wavelength. The standards used are spectrally flat over a wide wavelength range. Supplemental information is available for some materials with slope in their reflectance curves.*

Twelve Step Single Beam Substitution Error Correction Table (Part 1)

Wavelength	**Gray 0/S**	Gray 0/D	**Gray 4/S**	Gray 4/D	**Gray 5/S**	Gray 5/D	**Gray 7/S**	Gray 7/D	**Gray10/S**	Gray10/D	**Gray11/S**	Gray11/D
300	**0.009**	0.011	**0.053**	0.065	**0.099**	0.123	**0.192**	0.231	**0.337**	0.394	**0.378**	0.436
325	**0.009**	0.011	**0.050**	0.064	**0.095**	0.121	**0.188**	0.230	**0.329**	0.392	**0.371**	0.434
350	**0.009**	0.012	**0.050**	0.064	**0.093**	0.121	**0.184**	0.230	**0.323**	0.388	**0.366**	0.432
375	**0.009**	0.011	**0.049**	0.064	**0.092**	0.122	**0.182**	0.229	**0.319**	0.387	**0.362**	0.431
400	**0.010**	0.011	**0.048**	0.064	**0.091**	0.122	**0.181**	0.230	**0.316**	0.386	**0.360**	0.431
425	**0.010**	0.011	**0.048**	0.064	**0.091**	0.122	**0.181**	0.231	**0.314**	0.385	**0.359**	0.431
450	**0.010**	0.011	**0.048**	0.064	**0.091**	0.122	**0.182**	0.232	**0.313**	0.385	**0.358**	0.432
475	**0.010**	0.011	**0.049**	0.064	**0.091**	0.122	**0.183**	0.233	**0.313**	0.385	**0.359**	0.433
500	**0.010**	0.011	**0.049**	0.064	**0.092**	0.123	**0.184**	0.235	**0.313**	0.385	**0.359**	0.433
525	**0.010**	0.011	**0.050**	0.065	**0.092**	0.123	**0.186**	0.236	**0.313**	0.385	**0.360**	0.434
550	**0.010**	0.011	**0.050**	0.065	**0.093**	0.123	**0.187**	0.238	**0.313**	0.385	**0.361**	0.435
575	**0.010**	0.011	**0.050**	0.066	**0.093**	0.124	**0.188**	0.239	**0.314**	0.386	**0.362**	0.436
600	**0.010**	0.011	**0.051**	0.066	**0.094**	0.124	**0.190**	0.240	**0.315**	0.386	**0.364**	0.436
625	**0.010**	0.011	**0.051**	0.066	**0.095**	0.125	**0.191**	0.241	**0.316**	0.386	**0.365**	0.436
650	**0.011**	0.011	**0.052**	0.067	**0.095**	0.125	**0.193**	0.243	**0.317**	0.386	**0.366**	0.437
675	**0.011**	0.011	**0.052**	0.067	**0.096**	0.126	**0.194**	0.243	**0.317**	0.386	**0.367**	0.437
700	**0.011**	0.011	**0.053**	0.068	**0.097**	0.126	**0.195**	0.245	**0.318**	0.387	**0.368**	0.438
725	**0.011**	0.011	**0.054**	0.068	**0.098**	0.127	**0.196**	0.245	**0.319**	0.388	**0.369**	0.439
750	**0.011**	0.011	**0.054**	0.068	**0.099**	0.127	**0.198**	0.246	**0.320**	0.388	**0.370**	0.440
775	**0.012**	0.011	**0.055**	0.069	**0.100**	0.128	**0.199**	0.247	**0.321**	0.388	**0.371**	0.440
800	**0.012**	0.011	**0.056**	0.069	**0.101**	0.129	**0.200**	0.249	**0.323**	0.391	**0.372**	0.440
825	**0.012**	0.011	**0.057**	0.070	**0.102**	0.130	**0.202**	0.249	**0.324**	0.391	**0.374**	0.442
850	**0.013**	0.011	**0.057**	0.071	**0.102**	0.131	**0.203**	0.251	**0.325**	0.391	**0.375**	0.442
875	**0.013**	0.012	**0.058**	0.072	**0.104**	0.132	**0.204**	0.251	**0.326**	0.391	**0.376**	0.442
900	**0.013**	0.012	**0.059**	0.072	**0.104**	0.133	**0.206**	0.252	**0.327**	0.391	**0.377**	0.441
925	**0.014**	0.012	**0.059**	0.072	**0.105**	0.133	**0.207**	0.252	**0.328**	0.391	**0.378**	0.441
950	**0.014**	0.012	**0.060**	0.072	**0.106**	0.134	**0.208**	0.252	**0.329**	0.391	**0.379**	0.442
975	**0.014**	0.013	**0.061**	0.073	**0.107**	0.134	**0.209**	0.254	**0.331**	0.392	**0.380**	0.443
1000	**0.014**	0.012	**0.061**	0.073	**0.108**	0.135	**0.210**	0.255	**0.332**	0.392	**0.381**	0.443
1025	**0.014**	0.012	**0.062**	0.075	**0.108**	0.135	**0.210**	0.256	**0.333**	0.393	**0.382**	0.443
1050	**0.014**	0.012	**0.062**	0.075	**0.109**	0.135	**0.211**	0.256	**0.334**	0.392	**0.383**	0.444
1075	**0.014**	0.012	**0.062**	0.075	**0.110**	0.136	**0.212**	0.257	**0.334**	0.394	**0.383**	0.444
1100	**0.015**	0.012	**0.063**	0.076	**0.110**	0.138	**0.213**	0.257	**0.336**	0.396	**0.385**	0.445

Twelve Step Single Beam Substitution Error Correction Table (Part 2)

Wavelength	**Gray14/S**	Gray14/D	**Gray16/S**	Gray16/D	**Gray18/S**	Gray18/D	**Gray20/S**	Gray20/D	**Gray22/S**	Gray22/D	**Gray23/S**	Gray23/D
300	**0.512**	0.571	**0.636**	0.691	**0.730**	0.773	**0.791**	0.825	**0.895**	0.912	**0.956**	0.964
325	**0.505**	0.571	**0.631**	0.691	**0.725**	0.774	**0.792**	0.827	**0.898**	0.915	**0.965**	0.971
350	**0.500**	0.569	**0.627**	0.692	**0.722**	0.775	**0.790**	0.829	**0.899**	0.917	**0.970**	0.975
375	**0.495**	0.568	**0.624**	0.691	**0.718**	0.771	**0.789**	0.827	**0.898**	0.917	**0.974**	0.978
400	**0.492**	0.568	**0.623**	0.692	**0.716**	0.774	**0.789**	0.832	**0.899**	0.918	**0.978**	0.983
425	**0.491**	0.567	**0.622**	0.693	**0.715**	0.775	**0.790**	0.833	**0.899**	0.918	**0.980**	0.985
450	**0.490**	0.568	**0.623**	0.693	**0.714**	0.774	**0.791**	0.833	**0.900**	0.920	**0.981**	0.986
475	**0.491**	0.568	**0.624**	0.695	**0.715**	0.775	**0.793**	0.835	**0.902**	0.921	**0.983**	0.987
500	**0.491**	0.569	**0.624**	0.696	**0.715**	0.776	**0.794**	0.836	**0.902**	0.921	**0.983**	0.987
525	**0.492**	0.570	**0.626**	0.696	**0.716**	0.775	**0.795**	0.837	**0.903**	0.922	**0.983**	0.988
550	**0.493**	0.570	**0.627**	0.698	**0.716**	0.777	**0.797**	0.839	**0.904**	0.921	**0.983**	0.988
575	**0.495**	0.570	**0.628**	0.698	**0.717**	0.776	**0.798**	0.840	**0.905**	0.924	**0.983**	0.987
600	**0.496**	0.571	**0.629**	0.698	**0.718**	0.776	**0.800**	0.840	**0.906**	0.923	**0.983**	0.988
625	**0.497**	0.572	**0.631**	0.699	**0.719**	0.777	**0.802**	0.841	**0.907**	0.924	**0.983**	0.987
650	**0.498**	0.572	**0.632**	0.699	**0.719**	0.776	**0.803**	0.841	**0.907**	0.926	**0.983**	0.988
675	**0.499**	0.572	**0.633**	0.701	**0.720**	0.777	**0.805**	0.843	**0.908**	0.924	**0.983**	0.988
700	**0.500**	0.574	**0.634**	0.702	**0.721**	0.778	**0.806**	0.843	**0.909**	0.925	**0.983**	0.988
725	**0.501**	0.575	**0.635**	0.702	**0.721**	0.776	**0.807**	0.844	**0.910**	0.926	**0.983**	0.988
750	**0.503**	0.576	**0.637**	0.703	**0.722**	0.778	**0.809**	0.845	**0.911**	0.926	**0.983**	0.988
775	**0.504**	0.575	**0.638**	0.704	**0.723**	0.778	**0.810**	0.846	**0.912**	0.926	**0.984**	0.987
800	**0.506**	0.576	**0.640**	0.704	**0.724**	0.777	**0.812**	0.846	**0.913**	0.931	**0.984**	0.990
825	**0.507**	0.578	**0.641**	0.704	**0.725**	0.777	**0.813**	0.848	**0.913**	0.930	**0.983**	0.988
850	**0.508**	0.578	**0.642**	0.704	**0.725**	0.777	**0.813**	0.848	**0.913**	0.930	**0.982**	0.990
875	**0.509**	0.578	**0.644**	0.705	**0.726**	0.778	**0.814**	0.848	**0.912**	0.929	**0.981**	0.988
900	**0.511**	0.578	**0.645**	0.706	**0.726**	0.779	**0.814**	0.851	**0.912**	0.930	**0.980**	0.988
925	**0.512**	0.579	**0.646**	0.707	**0.727**	0.781	**0.815**	0.851	**0.913**	0.930	**0.980**	0.987
950	**0.513**	0.579	**0.647**	0.709	**0.728**	0.781	**0.817**	0.851	**0.914**	0.930	**0.980**	0.988
975	**0.515**	0.579	**0.648**	0.710	**0.728**	0.781	**0.818**	0.851	**0.914**	0.931	**0.981**	0.989
1000	**0.516**	0.579	**0.650**	0.710	**0.730**	0.782	**0.820**	0.854	**0.916**	0.931	**0.981**	0.988
1025	**0.517**	0.580	**0.651**	0.711	**0.730**	0.781	**0.821**	0.854	**0.917**	0.932	**0.982**	0.986
1050	**0.517**	0.580	**0.652**	0.712	**0.729**	0.781	**0.818**	0.855	**0.912**	0.932	**0.976**	0.988
1075	**0.518**	0.582	**0.652**	0.713	**0.728**	0.783	**0.816**	0.854	**0.909**	0.931	**0.971**	0.986
1100	**0.519**	0.581	**0.654**	0.714	**0.729**	0.783	**0.817**	0.856	**0.910**	0.932	**0.972**	0.988

**Note: Tables are used for diffusely reflecting materials ONLY.*

An example of the use of the twelve step single beam substitution error correction tables is shown in Figures 7, 8, and 9. In these measurements, Labsphere SCS Spectralon color standards were measured using a dual beam spectrophotometer with a single beam sphere accessory and a double beam spectrophotometer with a double beam sphere accessory. In each case, the bottom curve represents the measured spectrum generated on the single beam sphere. The 'boxed' curve represents the corrected values using the look-up tables. The light curve is the actual reflectance of the standard as measured on the double beam system, using the substitution error correction tables, give an excellent correlation with actual double beam measurements.

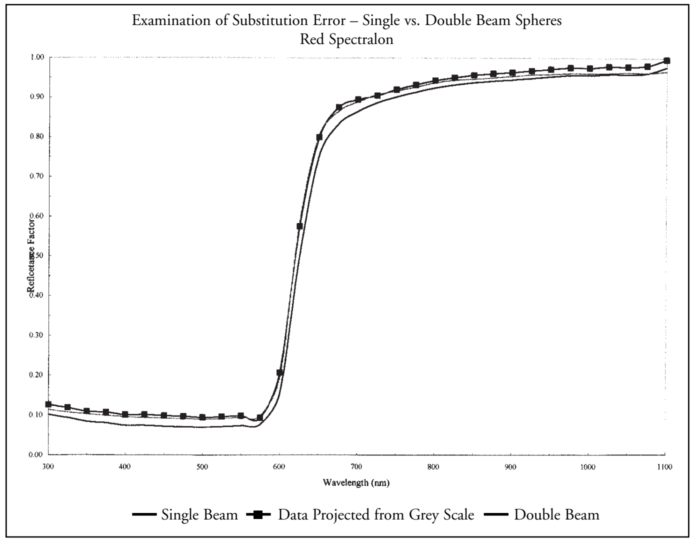

FIGURE 7

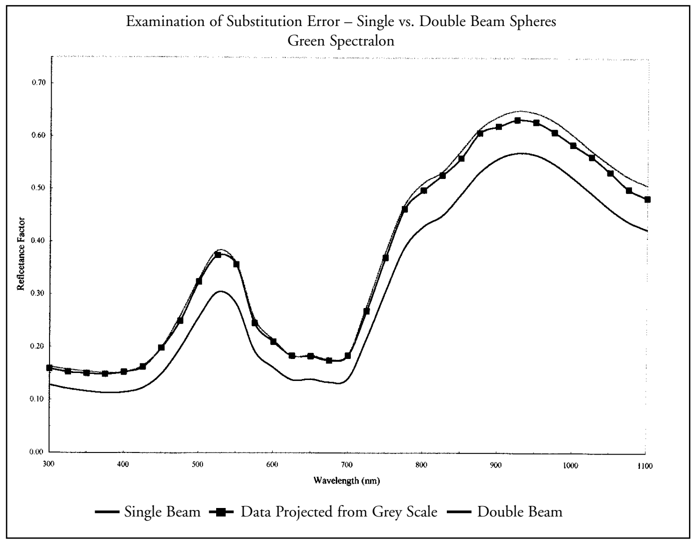

FIGURE 8

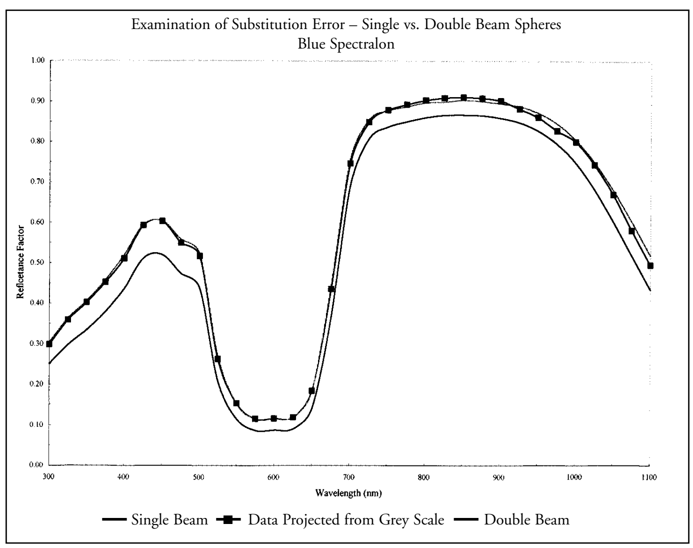

FIGURE 9

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UNITED STATES
Labsphere, Inc.
Tel: (603) 927-4266
Fax: (603) 927-4694
Email: labsphere@labsphere.com

GERMANY
Labsphere-Germany
Tel (49) 0 7556 50107
Fax: (49) 0 7556 50108
Email:labsphere@t-online.de

FRANCE
Labsphere-France
Tel: (33) 01 60 92 05 04
Fax (33) 01 60 92 04 95
Email: labsphere@wanadoo.fr

UNITED KINGDOM
Labsphere Ltd.
Tel: (44) 0 1625 871188
Fax: (44) 0 1625 871778
Email: labsphereltd@cs.com

0007-500