Software for the Absolute Correction Color Values and Calibration of Spectrometers, An Instrument Correction Program

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Abstract

We developed a software program that corrects known, systematic spectrophotometric errors seen in commercial spectrophotometers today. This enables users of spectrophotometers to correlate color values from around the world so that they will be nearly identical. This includes instruments manufactured by different manufacturers, and instruments manufactured by the same manufacturer. The program works on six different modalities; including bi-directional geometries; that is, 45°/0°; hemispherical, either d/0° or d/8° geometries; or multi-angle geometries. Multiangle geometries are used to characterize and assess gonioapparent inks and coatings. It is not necessary that both instruments be of the same geometry.

We summarize the performance of the software in the following statement: For modern instruments that are close in performance; that is less than 1 DE^*_{ab} one can expect that the errors will be reduced to an average of less than 0.10 DE^*_{ab} unit across 14 BCRA tiles. This agreement or correlation between two instruments can be relative; that is one instrument to another, or absolute; that is, correlating one or more instruments to a reference international standardization laboratory.

ISO[1] and CGATS.5[2] recommend methods to improve inter-instrument agreement. The software uses traceable artifact standards to do the training. Implementing this program allows conformance to in-house certification programs, ISO requirements, and CGATS. This is of particular importance to those who utilize ICC profiling.

The program is designed to be readily incorporated into your existing software. There are multiple implementation methodologies available. For instance; it can be incorporated into your existing software through a DLL, Dynamic Linked Library. It can be used externally in post processing modes with an MS Excel spreadsheet, or it is available in a full-featured, customizable, quality control package. This program operates transparently to the user. Included with the software are all the support programs and documentation required to utilize this application.

Introduction

The authors are professionally engaged in the instrumental measurement of color. The correlation of instrumental measurements is desired and yet has been elusive. There are at least five situations where improvement of instrumental spectrometer values would be beneficial.

The first case involves customers with multiple manufacturing sites. In this case, customers want identical color values from multiple color measuring spectrometers around the globe so that data can be compared and analyzed. In many industries manufacturing facilities are off-shore while the central laboratories are located in the US, for instance.

The second case involves customers, who in this business climate of corporate acquisition acquire companies that have spectrometers of different modalities. For instance; there are six popular modalities; SIN,[3] SEX,[4] d/8°,[5] d/0°,[6] 45°/0°,[7] & multi-angle.[8] Not included are a plethora of non-standard modalities. It is desirable to correlate values from any instrument with any modality to those values generated by a central laboratory instrument.

The third case is customers who have large product databases. In this case, the customer wants to preserve the integrity of the database. Often they are told that the database has to be "scrapped" because the values obtained with the new instrumentation do not correlate with the values obtained with the old instrument. Utilizing the old database values with the new instrumentation enables them to utilize standardized methods without introducing confusion.

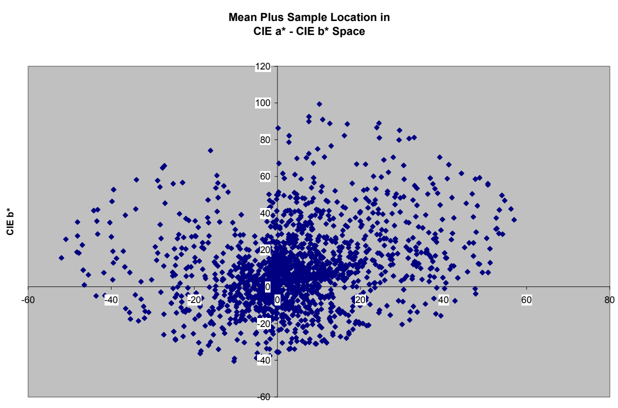
The fourth case involves customers who utilize a single universal database. Colorant manufactures and large manufacturers require data compatibility from around the globe as they use the colorant information for computer color matching and product colorization.

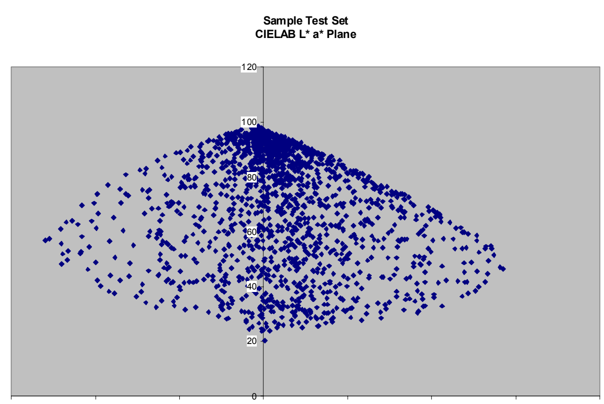
The fifth case involves companies who regularity utilize computer color matching or batch correction. These colorizing methods involve the preparation of multiple calibrations (let downs) for each colorant in a formula. Typically 3 to 6 colorants will be used to create each color. In this case the K/S values are calculated from measured spectral reflectance values at each wavelength. The K represents the absorption component of the mixture and the S represents the scattering component of the mixture. A form of Kubelka-Munk[9] equations uses these values to compute the desired pigment concentrations.

Statistical studies of the customer's databases for these cases show a weak correlation between different modalities, configurations, and different manufacturer's instruments. A model that could provide such a vehicle is of interest to the color community and has commercial value. Today as we engage in globalization and standardization; such as ISO, correlation becomes increasing important. The ability to utilize digital color values transmitted over the internet "Business @ the Speed of Thought"[10] has enormous competitive advantage by shortening the supply chain and reducing the time to market.

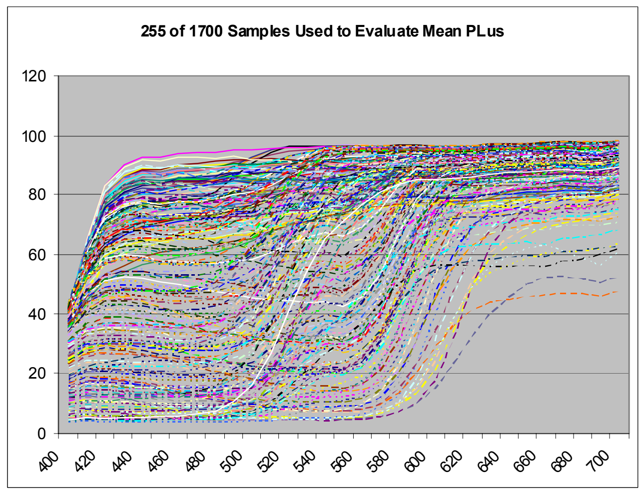
Experimental Modeling

The parameters for the proprietary algorithm and their coefficients were put together in a computer program that allowed us to input data; such as a database or library, process that data, and analyze the results generated by the executable program. This allowed us to validate and adjust empirically if necessary the results the program thereby optimizing the results. The results of the executable program are reported in two sets of specimens. The first set consists of < 1700 samples representing a library sampling a large portion of color space. The distribution of samples in color space is shown in Figure 1. This figure are the CIELAB data of the library plotted in the a* - b* plane of CIELAB color space. The same sample set is shown in Figure 2 in the L* versus a* plane. The library samples most of color space extensively. We then plotted the spectral reflectance factor and Figure 3 shows the distribution of 255 samples. The quantity of samples presented is a limitation of MS Excel.



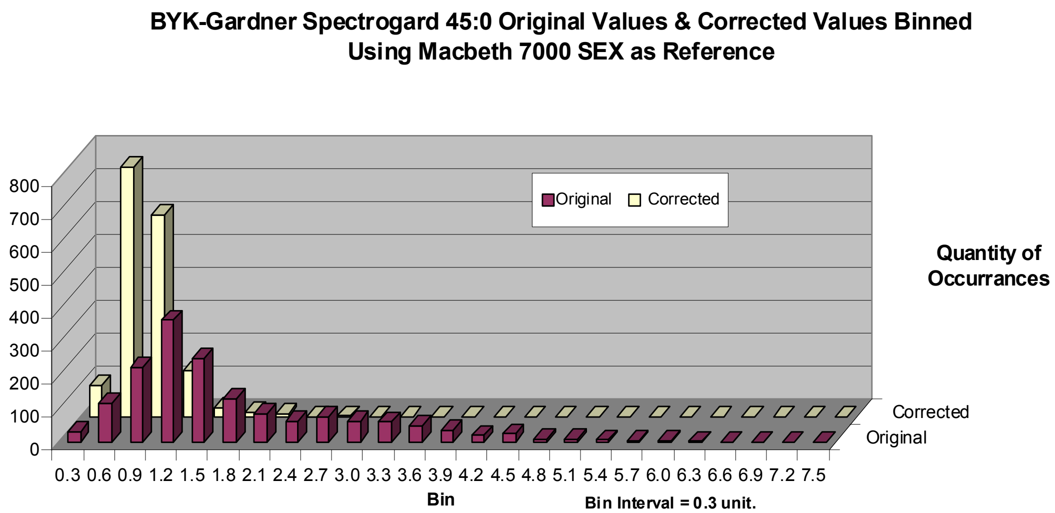


It is seen that the sample set contains high chroma samples. Samples with high chroma are difficult specimens to measure and correct because a small variation in the step slope of the reflectance curve causes a large error in CIELAB color space. The sample set contained a large number of neutral and near neutral samples. These samples tested the efficacy of the photometric correction. The surface finish on the sample set is primarily matte. The samples are paint applied on a stiff paper substrate. There were no special precautions taken when performing the measurement of the library. The measurements were performed by experienced operators and those skilled in the art. The instruments were standardized at regular intervals throughout the measurement process in accordance with manufacturer's recommendations. All the measurements of a library on one instrument were made in one day. The measurements were performed under reproducibility conditions. That is; different operators, different sample sets, different locations, and different instruments performed on different days. Reproducibility data are the most difficult type of data to correlate since all known variables need to be considered.



The effectiveness of this algorithm was tested by comparing values obtained using to industrial spectrometers, the Macbeth (MCB) 7000 and the BYK-Gardner (BG) Color View. The MCB is a D/8° sphere operating in the SEX modality with a 10 nm bandwidth instrument reporting from 360 to 780 nm, with a 30 mm LAV aperture. The BG instrument is a 45°: 0° geometry, LAV 25 mm aperture reporting from 400 to 700 nm with a 10 nm bandwidth at 10 nm intervals. The spectral bandwidth and center band frequency are not constant over the wavelength region interest.

Both the instruments use a white tile for standardization supplied by the manufacturer, and were standardized according to manufacturer's instructions. The manufacturers' calibrations are traceable to different national standardizing the laboratories, resulting in significantly different full scale 100 percent settings, approximately 2%. No other adjustments to the spectrometers were performed. The spectral reflectance factor data for each sample was collected and analyzed by another program in MS Excel that converts the data from spectral reflectance values to CIELAB values for the CIE 10° Observer Function under Illuminant D65.



We analyzed the resultant data by a technique called binning. That is, we created bins or buckets of 0.3 units CIELAB DE* from 0.00 to the maximum value. For the first bin we counted the number of samples whose values are between 0.00 and <0.29 unit. For the second bin we counted the number of samples whose values were >0.30 to < 0.59 unit, and so forth up to the maximum value. This is the data reported for the uncorrected values. In this case we "trained" the BG Color View to emulate the MCB 7000 unit. The program could perform the reverse correlation; that is correlating the BG Color View to the MCB 7000 as well with similar results. The results are shown graphically in Figure 4.

The data shows that in the corrected state > 90% of the samples are in bins less than 1.2 units with a maximum value of 2.7 units. This is contrasted to the uncorrected state where ~ 90% of the samples are contained in bins less than 3.3 units with the maximum being 6.6 DE^*_{ab} units.

Applications

The applications for this program are applicable to those who measure color in a variety of applications who are searching for an implementation method, a different method, or a different business model. This program will correct reported values by instruments made by different manufacturers, improve performance of instruments made by the same manufacturer, allow cross instrument modalities to be correlated, correct existing data bases to conform to new instrumentation values, and allow customers to preserve existing databases. This program is appropriate for color measurement of objects color; such as, inks, paints, plastics, and textiles.

Conclusion

The model for the correction of absolute spectrophotometric errors has been developed using numerical methods and proprietary modeling techniques. The correction model is based in large part of the work that was begun in the 1980s'. The math model deployed shows that systematic effects for known errors can be substantively reduced. The model shows that errors occurring in inter-instrument agreement, between a manufacturer's family of instruments; instruments of different modalities; and intra-instrument agreement, different manufacturer's instruments, can be substantially reduced thus providing the close agreement within or between factories around the globe.

The algorithm compensates for variances that occur as a result of design, calibration, and manufacturing. The sources of error include; specular port error, photometric full scale error, photometric zero error, photometric non-linearity, wavelength band pass, wavelength bandwidth, and sample aperture size.

The model does not improve imprecision in the form of repeatability of an instrument or translucency blurring,[11] an effect found in translucent materials. Improved correlation is shown between sampling apertures of different sizes used on the same instrument. These apertures sizes are called Large Area View, LAV, & Small Area View, SAV.

This model has performing well in industry for over three years.

References

1. ISO 13655 – ISO Central Secretariat, 1 rue de Varembe – CP 56, 1211 Geneva 20 Switzerland
2. CGATS, NPES,The Association for Suppliers of Printing , Publishing and Converting Technologies, 1899 Preston White Drive, Reston, Virginia 20191-4367
3. SIN is an acronym for Specular Included modality
4. SIN is an acronym for Specular Included modality
5. D/0o refers to diffuse illumination, viewing at 0 degrees relative to the sample normal. See ASTM 1331for a complete explanation. ASTM International, West Conshohocken, PA USA
6. D/8o refers to diffuse illumination, viewing at 8 degrees relative to the sample normal. See ASTM 1331for a complete explanation. ASTM International, West Conshohocken, PA USA
7. 45/0o refers to bidirectional geometry. Refer to ASTM E 1349 for a complete explanation. ASTM International, West Conshohocken, PA USA
8. Multi-angle refers to instrumentation designed to characterize and measure gonioapparent coatings. See ASTM E 2194 for a complete explanation. ASTM International, West Conshohocken, PA USA

9. Judd & Wyszecki, Color in Business, Science & Industry, Second Edition John Wiley & Sons, New York, 1952
10. Business @ the Speed of Thought, Bill Gates, Warner Books, May 2000.
11. Spooner, D.L. Translucent blurring errors in small area reflectance spectrophotometer & densitometer measurements. In: TAGA Proceedings 1991. Rochester, New York, USA: RIT Research Corporation, 1991. pp. 130–14

Author Biography

Jack Ladson currently is a principle in Color Science Consultancy. For twenty-five years Ladson has worked in the field of color and appearance technology. His current interests are in digital color technology, digital imaging, spectrophotometry & colorimetry, and global color control. He has had extensive experience at high levels in many aspects of business, including: R&D, Operations, and Sales & Marketing.

Ladson studied Optics at the University of Rochester and Mathematics at the Massachusetts Institute of Technology.

Ladson is actively involved in the Inter Society Color Council, and is the immediate past –president. He is an active member of the American Society for Testing and Materials (ASTM). He chairs the sub-committee ASTM E12.02 on Colorimetry and Spectrophotometry, E12.06 on Digital Imaging, and is task group chairman of Effect Coatings (Metallic and Pearlescent). He is actively involved in the committee on the Multidimensional Characterization of Appearance, Color Ordering Systems, Color Rendering and Visual Methods. He is a representative on Optical Properties of Plastics to the International Standards Organization (ISO). He is a member of: the United States National Committee - Commission Internationale de l'Eclairage (CIE); the Council on Optical Radiation Measurement, (CORM); American Association of Textile Chemist & Colorists, (AATCC), Detroit Color Council, (DCC), the American Statistical Association, (ASA); and the American Society for Quality, (ASQ).

Ladson has published over 30 papers on color; including digital imaging, color appearance phenomena, instrumental performance and process control. He is a co-author of color educational programs, Leonardo2000 and COMIC III. He is an invited lecturer in the US, Europe, and Asia. He has spoken (invited speaker) at meetings conducted by the ISCC, AIC, AATCC, DICOM (Medical Imaging), Cosmetic Conferences, Analytical Symposiums, Color Design Seminars, and Web Based Imaging Seminars.

Ladson consults for many industrial, international companies & businesses including Estee Lauder, BYK-Gardner, Datacolor International, P&G, LOF, Duha Color, Coronado Paint, Revlon, Coty, PPG, Color Science Corporation, Ballou Technologies, E-Color, Hoechst, Kansai Paint, BASF, Seradyn, and many more. His accomplishments include increasing sales by 15%, increasing factory capacity by 33%, increasing product quality 2 times, and reducing quantity of pigments by 69% by rationalizing. These were accomplished by using Lean Manufacturing methodologies and 6 Sigma quality tools.

He has been awarded patents for color technology related discoveries. He served as an advisor for 5 years to the PENN State Advisory Board on Nanoparticles. Ladson enjoys deploying new technologies to solve customer's needs.