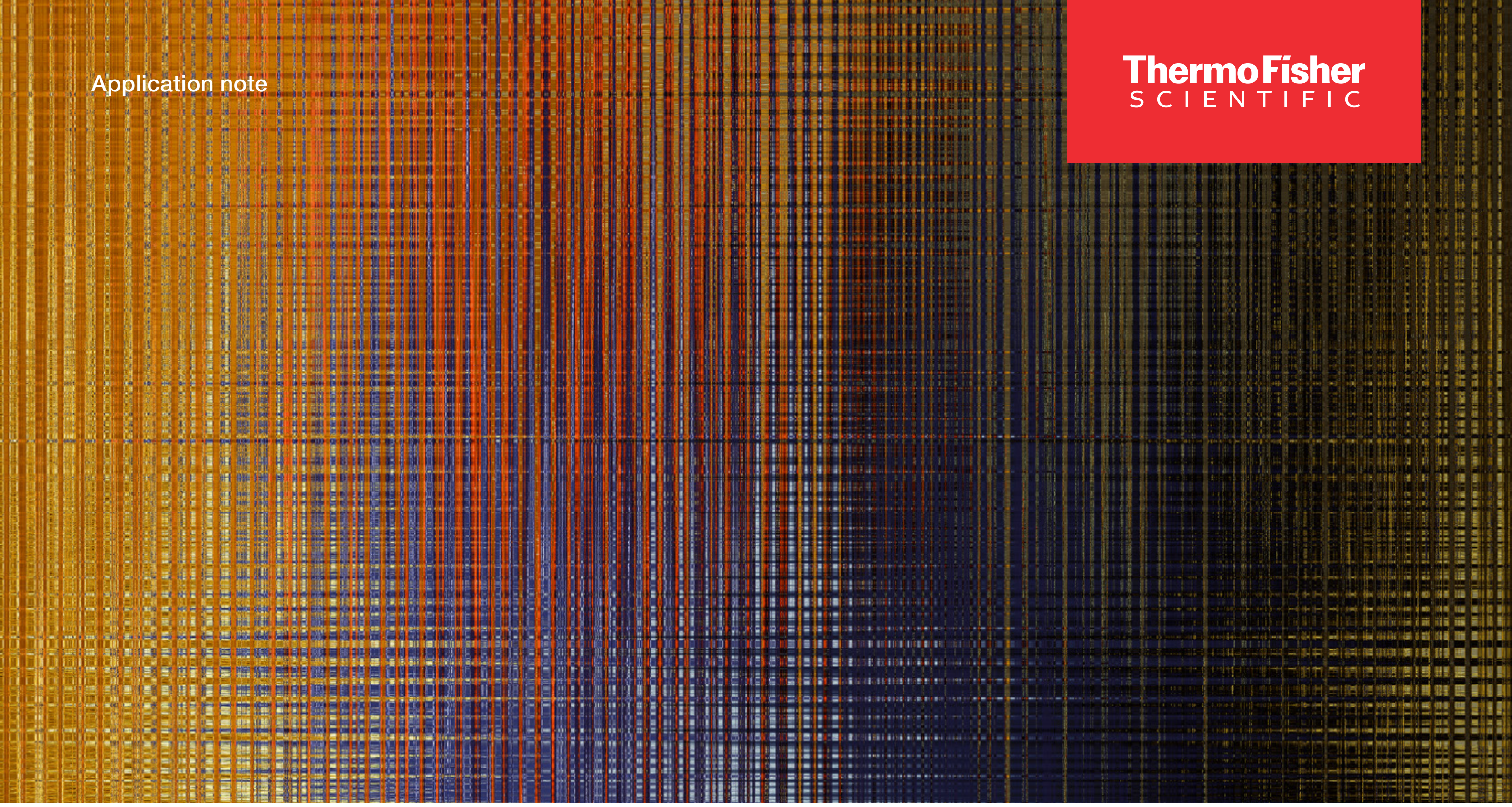

Application note

Utilizing UV-Visible Spectroscopy for Color Analysis of Fabrics

Introduction

The electromagnetic spectrum covers a wide range of energy from radio waves (low energy) to X-rays (high energy). The naked human eye can only see the visible region of the spectrum, covering wavelengths from 400 to 700 nm. Within that range, the light that reflects off an object into our eyes gives a material its color. Around 700 nm is where people visualize red; blue/purple is visualized around 400 nm (Figure 1).

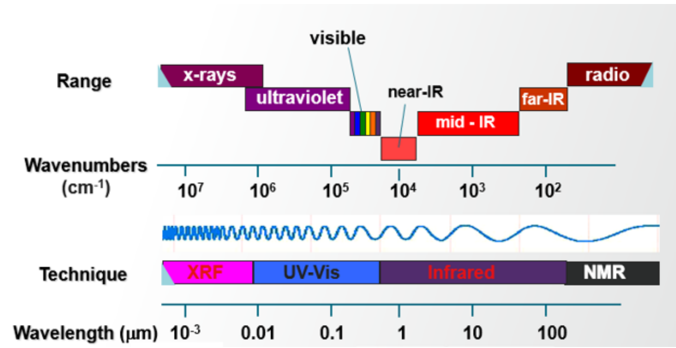

Figure 1. Electromagnetic radiation spectrum with corresponding spectroscopic techniques.

The color of a material has important implications when it comes to QA/QC in a wide range of industries, including the textile sector. One such example is studying environmentally friendly dyes that can be used in defensive camouflage within a combat background. In this situation the color of the textiles is designed to match the color of the woodland and plant environment.[1]

With fabrics, environmental factors such as light, oxygen and moisture can lead to degradation of the material. An important quality in relation to the dye used on the fabrics is color "fastness", or the resistance of a dye to fade or run. While such changes can be visualized with the human eye, there is no uniformity from person-to-person for such assessments. As a result, there is a desire to have a technique to quantify a material's color.[2]

UV-Visible spectroscopy has evolved to quantify the color of materials. The American Society for Testing and Materials (ASTM) outlines mathematics to assign a sample's color via coordinates on a graphical representation of color, or a color space.[3] The color space is developed by the Comission Internationale de l'Eclairage (CIE) using equations 1-3 to calculate the tristimulus values, X, Y, and Z, where $R(\lambda)$ represents the measured reflectance, k is a normalization factor, $S(\lambda)$ is the spectral power of the illuminant, and $\bar{x}(\lambda), \bar{y}(\lambda), \bar{z}(\lambda)$ are the color matching functions.

$$X = \sum_{400}^{700} k * S(\lambda) * \bar{x}(\lambda) * R(\lambda)\Delta\lambda \qquad (1)$$

$$Y = \sum_{400}^{700} k * S(\lambda) * \bar{y}(\lambda) * R(\lambda)\Delta\lambda \qquad (2)$$

$$Z = \sum_{400}^{700} k * S(\lambda) * \bar{z}(\lambda) * R(\lambda)\Delta\lambda \qquad (3)$$

The color of a material depends on factors such as the light source or the angle of view. The spectral power of the illuminant factors in different intensities of light sources (such as room lights or daylight) as a function of wavelength, accounting for how different light intensities can affect how color is perceived. The color-matching functions take into account the observer angle. As such, there are different illuminants and observer angles considered in calculating CIE tristimulus. For example, D_{65} at 10 degrees uses D_{65} illuminant, which simulates daylight, at an observer angle of 10 degrees.

CIE utilized these tristimulus values to create coordinates on uniform, cylindrical or spherical coordinate systems. The spherical system is represented by *CIE* $L^*_{a^*b^*}$ and the cylindrical has the coordinates *CIE* $L^*C^*_{h^*}$, each described in equations 4-8.

In equations 4-8 the X , Y , and Z represent the tristimulus values and X_n , Y_n , Z_n and are the tristimulus values of a perfectly reflecting white diffusor. L^* represents how light or dark a sample is, ranging from 100 being the lightest to 0 being the darkest. a^* represents how red or green an object is. A positive value represents red on the color space, while a negative value would represent green. b^* is yellow (positive) to blue (negative) (Figure 2).[1]

$$L^* = 116\left(\frac{X}{X_n}\right)^{\frac{1}{3}} - 16 \qquad (4)$$

$$a^* = 500\left[\left(\frac{X}{X_n}\right)^{\frac{1}{3}} - \left(\frac{Y}{Y_n}\right)^{\frac{1}{3}}\right] \qquad (5)$$

$$b^* = 200\left[\left(\frac{Y}{Y_n}\right)^{\frac{1}{3}} - \left(\frac{Z}{Z_n}\right)^{\frac{1}{3}}\right] \qquad (6)$$

$$C^*_{ab} = \sqrt{a^{*2} + b^{*2}} \qquad (7)$$

$$h^*_{ab} = \tan^{-1}\left(\frac{b^*}{a^*}\right) \qquad (8)$$

CIE $L^*C^*_{h^*}$ uses the same coordinates but instead uses chroma, C^*_{ab}, and hue, h^*_{ab}. Chroma quantifies how colorful a substance is, with a low value being pale to a high value being vibrant. Hue represents the color of the material.

When comparing the color of different materials, the color difference, ΔE^*_{ab}, is used via the equation 9, where ΔL^*, Δa^* and Δb^* represent the differences in the respective color values (L^*, a^*, and b^*) between the sample and the reference material.

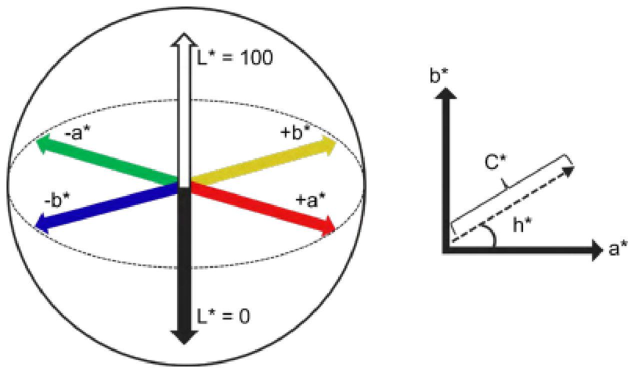

Figure 2. ***CIE*** $L^*_{a^*b^*}$ **(left) and** ***CIE*** $L^*C^*_{h^*}$ **(right) coordinates**

When there is a $\Delta E^*_{ab} < 3$ the two colors are considered indistinguishable when viewed by the human eye. These CIE values have been applied to ISO standards in measuring color fastness in textiles.[2]

$$\Delta E^*_{ab} = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2} \qquad (9)$$

In this note, the color of different fabrics and dyes commonly used with textiles were analyzed using the Thermo Scientific™ Evolution™ One Plus UV-Vis Spectrometer along with the Thermo Scientific™ Insight™ Pro Software. Here the CIE values of two different fabrics of similar color were compared to reveal subtle differences that may not be easily detected by eye. In addition a Thermo Scientific™ Nicolet™ iS20 FTIR Spectrometer was used to determine the fabric chemical composition.

Experimental

Materials

Three sets of materials were studied to give examples of color analysis via UV-Vis spectroscopy. One set contained three direct dyes: Direct Blue 71, Direct Red 81, and Direct Yellow 27. Direct dyes are used on cotton fabrics due to their ability to bond well with cellulose based material.[4] The dyes were dissolved in distilled water at concentrations of 2.5×10^{-6} M, 2.5×10^{-6} M and 1.25×10^{-5} M for red, blue and yellow, respectively, to produce absorption values of less than 1 (Figure 3).

Two sets of fabrics were analyzed, one of pure cotton and the second set of pure polyester. Since these fabrics were obtained commercially, Fourier Transform Infrared (FTIR) spectroscopy was performed to confirm the materials of the fabrics. Each set of fabrics had six colors tested: white, black, red, blue, yellow and green by appearance; these are represented by samples 1c through 6c for cotton and 1p through 6p for polyester, in that order (Figure 4).

Instrumental Analysis

The UV-Visible absorption spectra of the dye solutions were collected using the Evolution One Plus Spectrometer. Data was collected from 780 nm to 380 nm at a bandwidth of 1 nm, a data interval of 1 nm, and an integration time of 0.30 seconds.

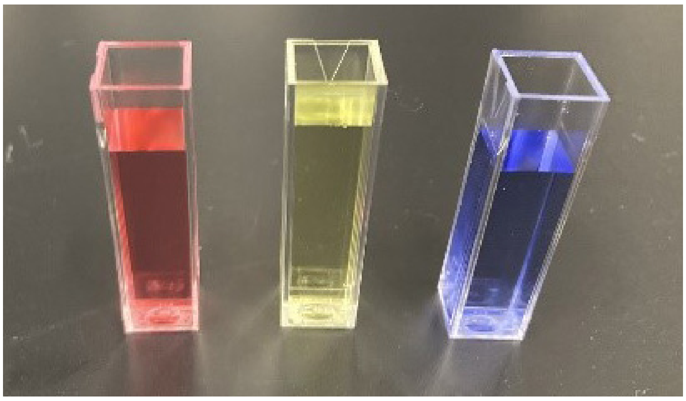

Figure 3. Image of Direct Red 81 (left), Direct Yellow 27 (middle) and Direct Blue 71 (right) dissolved in water.

The UV-Visible reflectance spectra of the fabric samples were collected using the same spectrophotometer equipped with an integrating sphere (ISA-220) in reflection mode. The collection parameters were the same as those for the absorption measurements. The data was reported in % Reflectance (%R) where a white Spectralon disk was used as a blank.

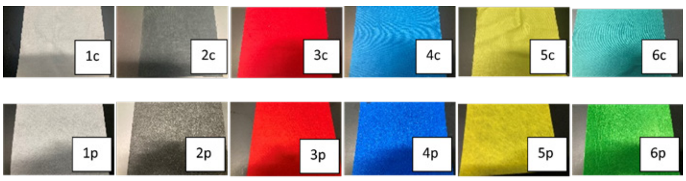

Figure 4. Top, cotton fabric. Botton, polyester fabric.

FTIR measurements were acquired using a Nicolet iS20 with an iTX diamond ATR accessory at 16 scans, at 4 wavenumber resolution. A library correlation search to identify the material was performed using Thermo Scientific™ Omnic™ Software.

Color analysis

The Insight Pro Software was used to calculate *CIE* $L^*_{a^*b^*}$ color values as described in USP <1061>[5] and ASTM-E308[3]. A D65 illuminant at a 10° observer angle was chosen.

Results and Discussion

Direct Dye Analysis

Three direct dyes were selected for analysis as these compounds are useful for coloration of fabrics consisting of cotton and cellulose. For synthetic material like polyester, disperse dyes are preferred.[4] However, in this note only direct dyes were analyzed.

The spectra for the three dyes are shown in Figure 5. As expected, the dyes absorb the visible light at their respective complementary colors with yellow absorbing at 400 nm, red absorbing at 512 nm, and blue at 586 nm.

Table 1 shows the *CIE* $L^*_{a^*b^*}$ values for each direct dye. In reference to Figure 2, coordinates *a** and *b** fall in line with each perceived color. (As described previously, red is represented by a positive *a**, yellow is a positive *b**, and blue is a negative *b**.)

Analysis of fabrics

Cotton and polyester fabrics were analyzed as well to determine if the material of the fabric will affect the calculated CIE color values. First, FTIR spectra were collected to confirm the fabric composition. As confirmed by FTIR library correlation search, the materials are cotton and polyester (Figure 6).

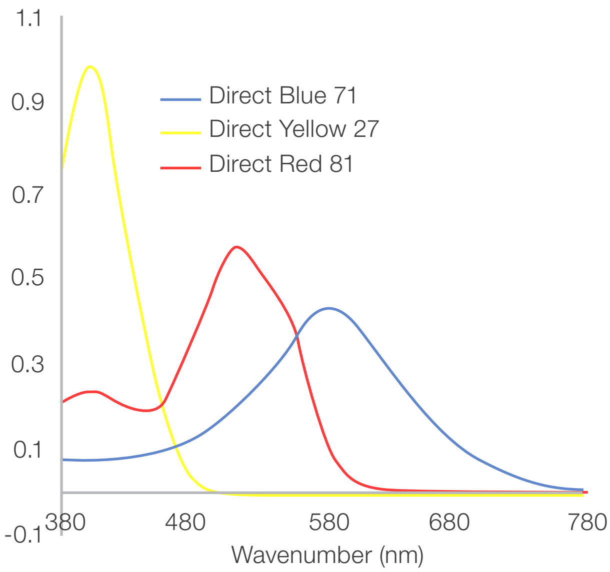

Figure 5. UV-Visible absorbance spectra of direct dyes.

Dye	L*	a*	b*
Direct Red 81	78.69	42.38	-3.16
Direct Yellow 27	99.69	-12.18	32.44
Direct Blue 71	77.27	0.06	-24.43

Table 1. CIE L*a*b* values for direct dyes.

Figure 7 includes the %R spectrum for each sample. Upon looking at the spectra, it is not straightforward to determine differences between each sample. However, using the *CIE* $L^*_{a^*b^*}$ color analysis the differences in color between each sample can be quantified. Table 2 and 3 shows the *CIE* $L^*_{a^*b^*}$ values for cotton and polyester, respectively. For cotton sample 1 the reflection close to the UV region is above 100%, which is likely a result of the white fabric being more reflective than the Spectralon standard. This is because reflective measurements are relative as opposed to being absolute measurements.

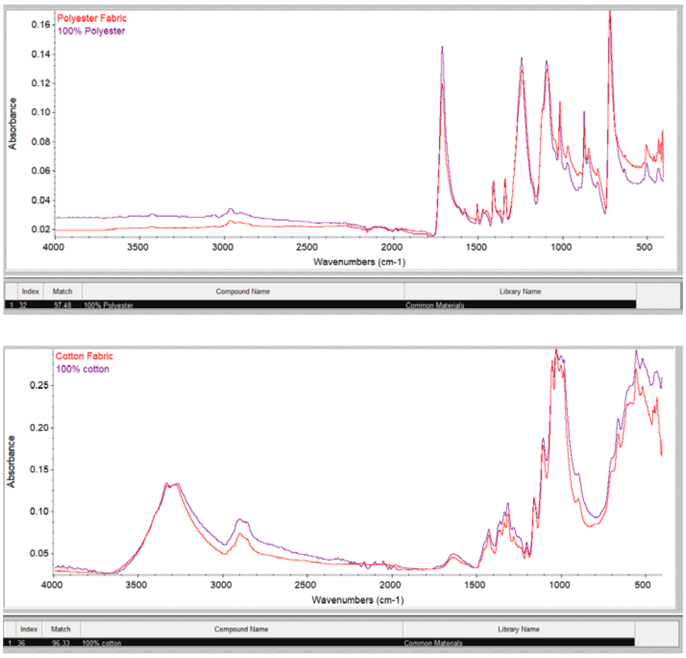

Figure 6. Spectrum of polyester (left) and cotton (right) fabrics. Red curve is the ATR data of the samples; the purple curve is the library correlation search.

As expected, regardless of the material analyzed, the color calculation falls in line with the perceived color. Samples 3c and 3p, the red fabrics, have positive *a** values, while samples 4c and 4p, the blue fabrics, have negative *b** values. Samples 5c/5p and 6c/6p appear yellow and green and thus have a positive *b** value and negative *a** value, respectively. Samples 1c/1p and 2c/2p, being white and black, have *a** and *b** values close to zero while their differences lie in the calculated *L** value.

In both tables 2 and 3 along with Figure 4, the two materials have similar CIE values with the exception of samples 6c and 6p. For cotton, the "green" sample (6c) chosen appeared the most green out of the fabric set.

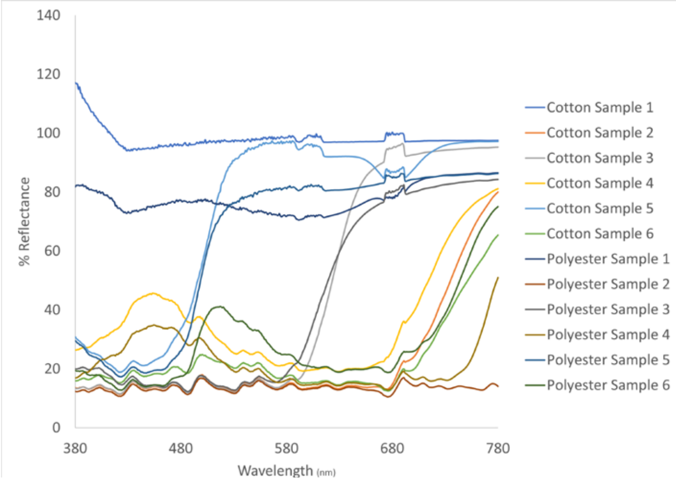

Figure 7. UV-Visible reflectance spectra of the cotton and polyester fabric samples

As seen visually, when compared to the green polyester sample (6p, Figure 4) there is a clear difference. This is also seen in the CIE values where the ΔE^*_{ab} value has the largest value. As mentioned earlier, a $\Delta E^*_{ab} < 3$ is discernable to the human eye. Table 4 shows the ΔE^*_{ab} for each sample with their respective color counterpart.

The biggest color difference observed is between the "green" cotton and polyester samples (samples 6c/6p) which is not surprising as they appear clearly different. Samples 2c/2p and 3c/3p are the closest in color where the quantified color difference. The *L** value for cotton sample 4 is higher compared to its polyester counterpart suggesting the cotton sample is a lighter shade. This is visually confirmed as shown in Figure 4. Similarly, the cotton fabric corresponding to sample 5 has a higher *L** value and appears by eye to have a lighter shade compared to the polyester fabric. If there is no difference in *L** between the two fabric materials, almost all (except sample 6) would have color differences of less than 3, indicating they are indistinguishable to the human eye. Therefore, for samples 4 and 5 the difference in appearance is primarily from the shade of the two fabrics and not the perceived color. The origin of the difference in the shades is out of the scope of this discussion.

Sample Cotton	L*	a*	b*
Sample 1	99.05	-0.32	1.51
Sample 2	44.80	-1.90	1.36
Sample 3	51.11	29.63	11.93
Sample 4	58.19	-3.34	-21.13
Sample 5	93.46	-6.12	61.34
Sample 6	51.07	-10.45	1.73

Table 2. *CIE* $L^*_{a^*b^*}$ values for the cotton samples.

Sample Polyester	L*	a*	b*
Sample 1	88.86	-1.74	-0.97
Sample 2	43.81	-1.34	1.74
Sample 3	53.12	30.74	12.84
Sample 4	51.92	-4.71	-19.22
Sample 5	87.84	-5.48	57.82
Sample 6	60.50	-24.45	-23.31

Table 3. CIE L*a*b* values for the polyester samples.

Sample	ΔE^*_{ab}	ΔE^*_{ab} with $\Delta L^* = 0$
Sample 1	10.58	2.58
Sample 2	1.20	0.68
Sample 3	2.47	1.43
Sample 4	6.70	2.35
Sample 5	6.66	3.58
Sample 6	30.20	28.69

Table 4. ΔE^*_{ab} of the cotton and polyester samples along with ΔE^*_{ab} when $\Delta L^* = 0$.

Conclusion:

Color analysis in materials is important to QA/QC in industry, especially the textile sector. With fabrics, this can apply to situations such as color fasting and camouflage in combat backgrounds, where the color differences may not be clearly distinguishable and may appear different to different people. Here, the Evolution One Plus UV-Visible spectrometer was used to determine the *CIE* $L^*_{a^*b^*}$ color values of different fabrics, revealing subtle differences between fabric materials that appear to be the same color by eye. Additionally, the quantification of different fabric dyes were performed using CIE color analysis, and the quantifications matched expected results. Also, FTIR measurements of both fabric types were collected and confirmed their anticipated chemical compositions. Through a combination of both UV-Visible and FTIR spectroscopic techniques, a robust QA/QC analysis can be achieved.

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