HOW TITANIUM DIOXIDE SELECTION CAN IMPROVE COLOR MATCHING PERFORMANCE AND FORMULATION CAPABILITY

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ABSTRACT

Titanium dioxide pigments offer the plastics industry attractive physical and optical performance characteristics. Tinting strength and undertone are quantifiable measurements of optical properties of titanium dioxide and pigment performance characteristics. These parameters provide opacification and brightness data to downstream consumers of titanium dioxide to allow them to appropriately develop formulations in combination with colored pigments to achieve a target specification in the color space. This paper describes the relationship between titanium dioxide optical properties of tinting strength and undertone and the resulting effect on chroma, hue and saturation within the color space. This relationship is crucial to understanding the impact of titanium dioxide grade differences and optical space analysis for color formulation and resulting product color performance.

Introduction

Tinting strength and undertone are two performance parameters that provide details of titanium dioxide grades and their end use optical performance characteristics. Tinting strength and undertone of the chosen grade of titanium dioxide contribute to the final color of the product.

The ability of titanium dioxide to selectively scatter certain wavelengths of light is a function of the pigment particle size diameter and distribution. The relationship of particle diameter to light scattering efficiency was first described by Rayleigh (Lilienfeld, 2004) and further refined by Mie (Mie, 1908), Horvath (Horvath, 2009), and Van de Hulst (Van de Hulst, 1981). The relationship between particle diameter and light scattering defines the maximum scattering efficiency of a particle as a function of the ratio between the particle diameter to wavelengths of light. Light scattering is most efficient when the particle is half the diameter of the wavelength of light it scatters. (Davis, Niedenzu, & Reid, 2010)

Tinting strength is controlled by the particle size distribution of titanium dioxide. A narrower distribution provides higher tinting strength as more particles will be appropriately sized, as described by Mie theory, for optimal scattering of light in the visible spectrum (Davis, Niedenzu, & Reid, 2010). The reflectance/scattering of titanium dioxide in a tinted system can be measured by mixing with black pigment to create a gray tinted system in polyvinylchloride. Monitoring the scattering intensity of the green wavelength in the gray plastic allows for determination of a tinting strength effect when compared to a standard to quantify the opacifying strength of the pigment.

Tinting strength requirements of titanium dioxide are application-dependent. A high tinting strength titanium dioxide is advantageous in fully opaque, bright white applications; for example, thin films where the scattering of light must occur in a thin cross-section prior to light passing through the product, minimizing visibility of the substrate. In exterior color applications, a lower tinting strength pigment can be advantageous to minimize the amount of colorant required to overcome the whiteness of titanium dioxide and reach the targeted product color while still providing appropriate levels of durability and UV stability performance. (Feng & Birmingham, 2003)

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The undertone of titanium dioxide pigments range from “cream” to “blue” and is a function of the mean particle size of the titanium dioxide grade. The average particle size of pigmentary titanium dioxide determines the scattering affinity of light across the visible spectrum. Mie theory explains that the optimum particle size for light scattering occurs when the particle is half the diameter of the wavelength of light it scatters.

Therefore, larger particles scatter yellow light more efficiently (longer wavelength in the visible spectrum) and provide a cream undertone, whereas smaller particles provide better scattering efficiency of blue light (shorter wavelength in the visible spectrum).

Consistent undertone of titanium dioxide is particularly important to colored products since variation in titanium dioxide undertone can have a large impact on the final product color.

Therefore, larger particles scatter yellow light more efficiently (longer wavelength in the visible spectrum) and provide a cream undertone, whereas smaller particles provide better scattering efficiency of blue light (shorter wavelength in the visible spectrum).

Figure 1. Tinting strength and undertone values in experimental grid

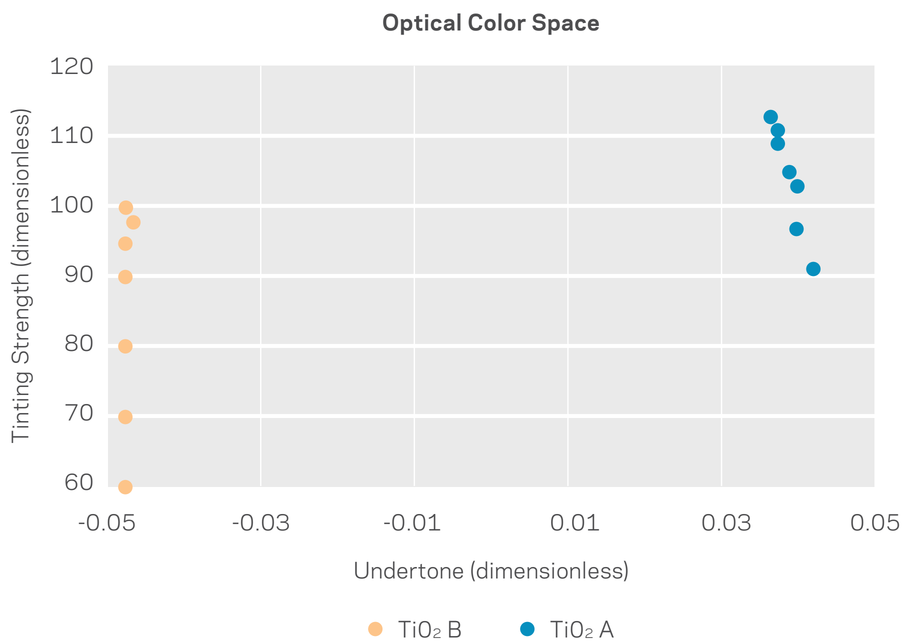
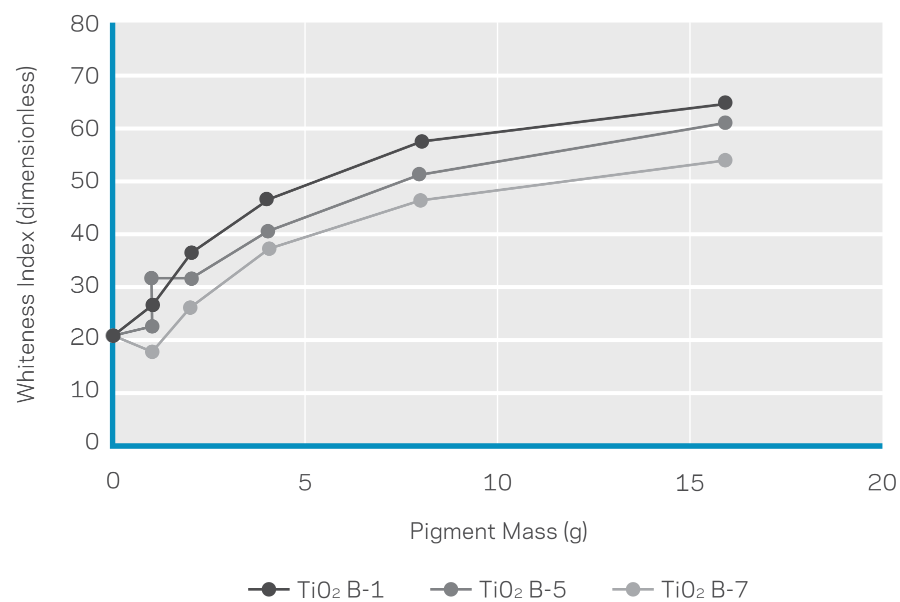


Figure 2. Effect of tinting strength and pigment loading on the whiteness index of samples



Experimental

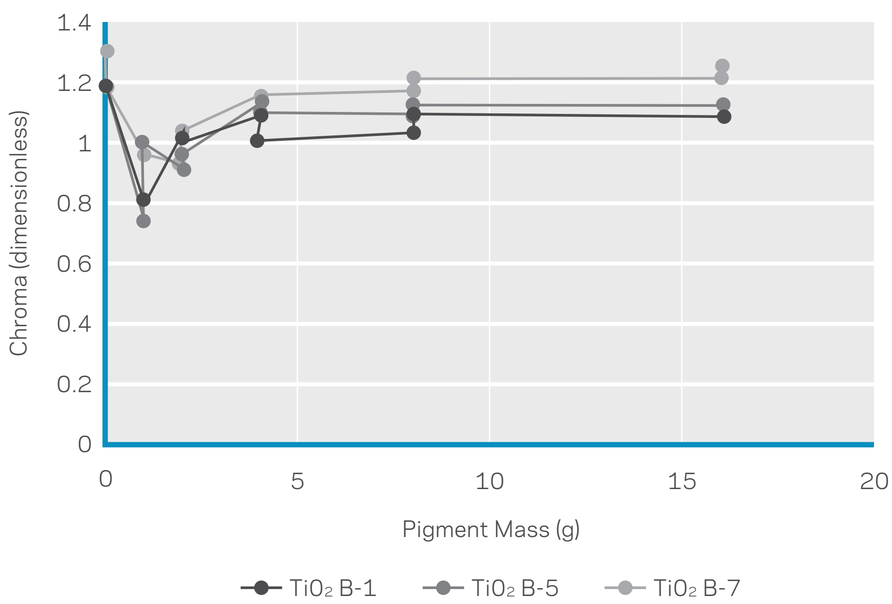
The purpose of this work was to evaluate the impact of titanium dioxide grades having different tinting strengths on the color of a tinted product with consistent undertone, as well as a difference in titanium dioxide undertone while evaluating similar tinting strength performance. This was completed by analyzing laboratory-prepared blends of titanium dioxide pigments with different concentrations of Epsom salt ($MgSO4.7H2O$, refractive index 1.43) to achieve a varying degree of pigment opacification power. Epsom salt does not create a color center, but serves to dilute the hiding power of the titanium dioxide in the overall pigment blend.

Two grades of titanium dioxide, with differing median particle size, were chosen for this experiment: one grade with a blue (positive) undertone (TiO_2 A) and one with a cream (negative) undertone (TiO_2 B).

Table 1. Experimental grid of titanium dioxide/salt blends

Pigment	Sample ID	Pigment Mass (g)	Epsom Salt (g)
TiO_2 A	TiO_2 A-1	100	0
TiO_2 A	TiO_2 A-2	99	1
TiO_2 A	TiO_2 A-3	98	2
TiO_2 A	TiO_2 A-4	96	4
TiO_2 A	TiO_2 A-5	92	8
TiO_2 A	TiO_2 A-6	88	12
TiO_2 A	TiO_2 A-7	84	16
TiO_2 B	TiO_2 B-1	100	0
TiO_2 B	TiO_2 B-2	99	1
TiO_2 B	TiO_2 B-3	98	2
TiO_2 B	TiO_2 B-4	96	4
TiO_2 B	TiO_2 B-5	92	8
TiO_2 B	TiO_2 B-6	88	12
TiO_2 B	TiO_2 B-7	84	16

Figure 3. Figure 3. Effect of tinting strength and pigment loading on the chroma of samples (as measured by the difference between the sample and standard as described in a polar coordinate system)



By preparing samples with different concentrations of Epsom salt, evaluations were conducted comparing pigment blends with the same undertone but different tinting strengths, and pigment blends with similar tinting strengths but different undertones. This evaluation served to summarize the relationship between these two optical property measurements and the resulting effect on product color. The tinting strength and undertone of the pigment blends tested in these experiments are summarized in Figure 1 (p. 3).

Pigment blends were prepared in the laboratory by mixing the desired grade of titanium dioxide with varying concentrations of Epsom salt using a V-cone blender. The pigment blends were first analyzed for tinting strength and undertone values. Then, various sample sizes of select pigment blends were combined with one pellet of a 40% black masterbatch in polyethylene and a 1.9MI, 0.92 g/cc low density polyethylene resin on a two-roll mill and pressed to produce rigid plaques for additional optical evaluation and analysis. Blend concentration data are summarized in Table 1 (p. 4) and black masterbatch data are summarized in Table 2 (below).

Table 2. Pigment blends with black masterbatch: sample preparation

Pigment	Pigment Mass (g)	Mass Polymer (g)	Black Masterbatch mass (g)
TiO_2 0	0	190	0.0266
TiO_2 A-1	1	189	0.0260
TiO_2 A-1	2	188	0.0266
TiO_2 A-1	4	186	0.0274
TiO_2 A-1	8	182	0.0260
TiO_2 A-1	16	174	0.0261
TiO_2 A-5	1	189	0.0263
TiO_2 A-5	2	188	0.0269
TiO_2 A-5	4	186	0.0278
TiO_2 A-5	8	182	0.0265
TiO_2 A-5	16	174	0.0277
TiO_2 A-7	1	189	0.0262
TiO_2 A-7	2	188	0.0261
TiO_2 A-7	4	186	0.0264
TiO_2 A-7	8	182	0.0267
TiO_2 A-7	16	174	0.0268

Continued at right...

Pigment	Pigment Mass (g)	Mass Polymer (g)	Black Masterbatch mass (g)
TiO_2 B-1	1	189	0.0246
TiO_2 B-1	2	188	0.0239
TiO_2 B-1	4	186	0.0245
TiO_2 B-1	8	182	0.0243
TiO_2 B-1	16	174	0.0242
TiO_2 B-5	1	189	0.0263
TiO_2 B-5	2	188	0.0269
TiO_2 B-5	4	186	0.0278
TiO_2 B-5	8	182	0.0265
TiO_2 B-5	16	174	0.0277
TiO_2 B-7	1	189	0.0262
TiO_2 B-7	2	188	0.0261
TiO_2 B-7	4	186	0.0264
TiO_2 B-7	8	182	0.0267
TiO_2 B-7	16	174	0.0268

Results and Conclusion

The results of this experiment showed the different optical performance characteristics of the pigment blends by studying pigments with the same undertone but different tinting strengths, as well as similar tinting strengths but different undertones. The tinting strength and undertone values of the pigment blends used in this experiment are summarized in Table 3 (below).

Analysis of samples with similar undertone and different tinting strengths showed similar hue, chroma and yellow values as the pigment blend concentration was increased in the polyethylene/carbon black compound. However, the whiteness (saturation) of the samples increased with increasing levels of titanium dioxide in the pigment blend. Increasing the tinting strength of the pigment blend provided an increase of 25.2% in whiteness at 2.1% pigment in the compound. The effect of tinting strength on optical properties of the sample are displayed graphically in Figures 2, 3, 4 and 5 (pp. 3, 4, and 7).

Table 3. Tinting strength and undertone values of starting pigment blends

Sample ID	Pigment Concentration (%)	Tinting Strength	Undertone
TiO_2 A-1	100	113	0.027
TiO_2 A-2	99	109	0.028
TiO_2 A-3	98	111	0.028
TiO_2 A-4	96	105	0.029
TiO_2 A-5	92	103	0.030
TiO_2 A-6	88	97	0.030
TiO_2 A-7	84	91	0.032
TiO_2 B-1	100	100	-0.048
TiO_2 B-2	99	98	-0.047
TiO_2 B-3	98	95	-0.048
TiO_2 B-4	96	90	-0.048
TiO_2 B-5*	92	80	-0.048
TiO_2 B-6*	88	70	-0.048
TiO_2 B-7*	84	60	-0.048

Continued at right...

*Please note that due to samples sticking to rollers, blends B-5 through B-7 tinting strength and undertone were extrapolated from data collected on other pigment blends in the sample set.

The analysis of pigments with similar tinting strengths and different undertone values was also performed. The hue and yellowness values of the pigment blends showed significant differences as increased levels of pigment were used in the sample preparation. Chroma was substantially different at low pigment loading levels, but merged as additional pigment was added to the sample. The whiteness values (as measured by whiteness index) were offset due to slightly different tinting strength values, but showed similar results for pigments with different undertones. The results of the different undertone value pigments with similar tinting strengths are summarized in Figures 6, 7, 8 and 9 (pp. 8 and 9). These results reinforce the critical nature of choosing a titanium dioxide pigment that is designed for use in each application.

Increased tinting strength, resulting in higher hiding power, is advantageous in applications where high opacification requirements are desired, such as opaque film production.

Figure 4. Effect of tinting strength and pigment loading on the hue of samples (as measured by the difference in angle between the sample and standard as described in a polar coordinate system)

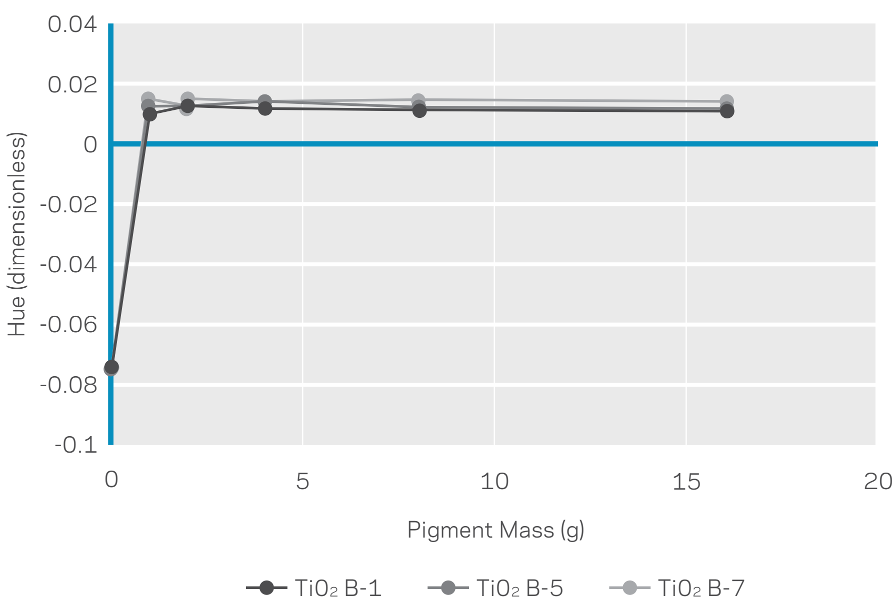
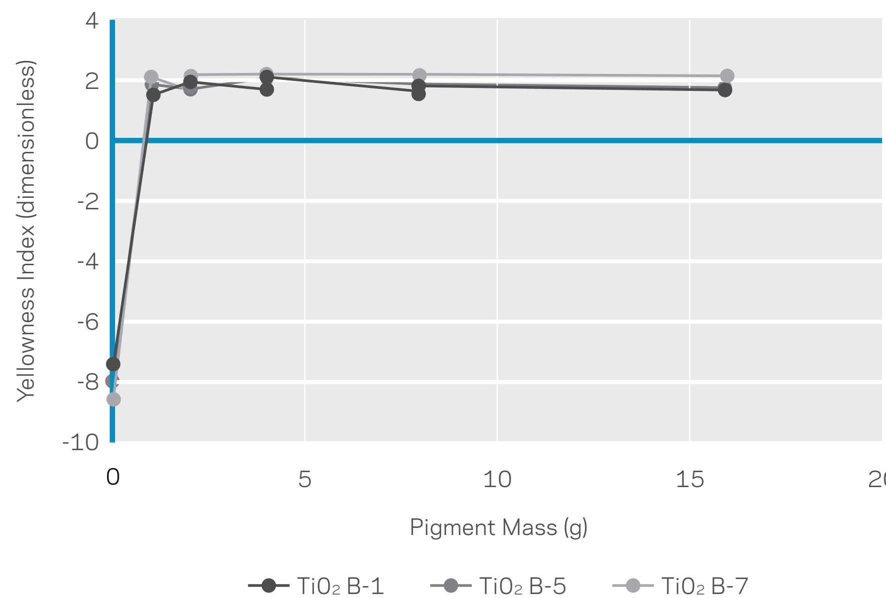


Figure 5. Effect of tinting strength and pigment loading on the yellowness index of samples



Increased tinting strength, resulting in higher hiding power, is advantageous in applications where high opacification requirements are desired, such as opaque film production. Lower tinting strength can be preferred in exterior color applications where ultraviolet light stability requirements are necessary, as a lower concentration of colorants can be required to overcome the whiteness provided by titanium dioxide.

Tinting strength and undertone are quantifiable measurements of optical properties of titanium dioxide and pigment performance characteristics within the overall color space. This work detailed changes in color space resulting from differences in tinting strength and undertone of titanium dioxide pigments. The relationship of tinting strength and undertone of titanium dioxide pigments and grade selection are crucial to establish consistent product color performance.

Figure 6. Effect of undertone and pigment concentration on the whiteness index of samples

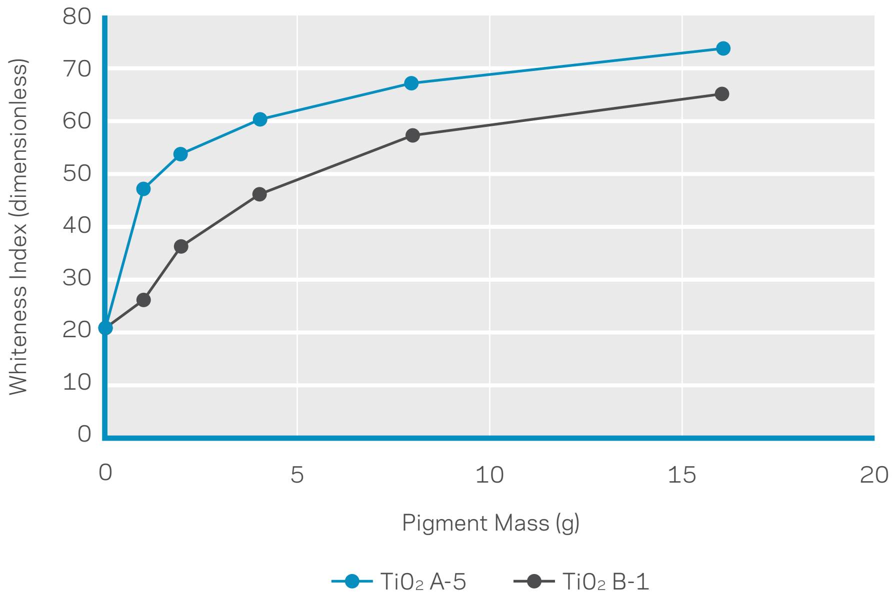


Figure 7. Effect of undertone and pigment concentration on the chroma of samples (as measured by the difference between the sample and standard as described in a polar coordinate system).

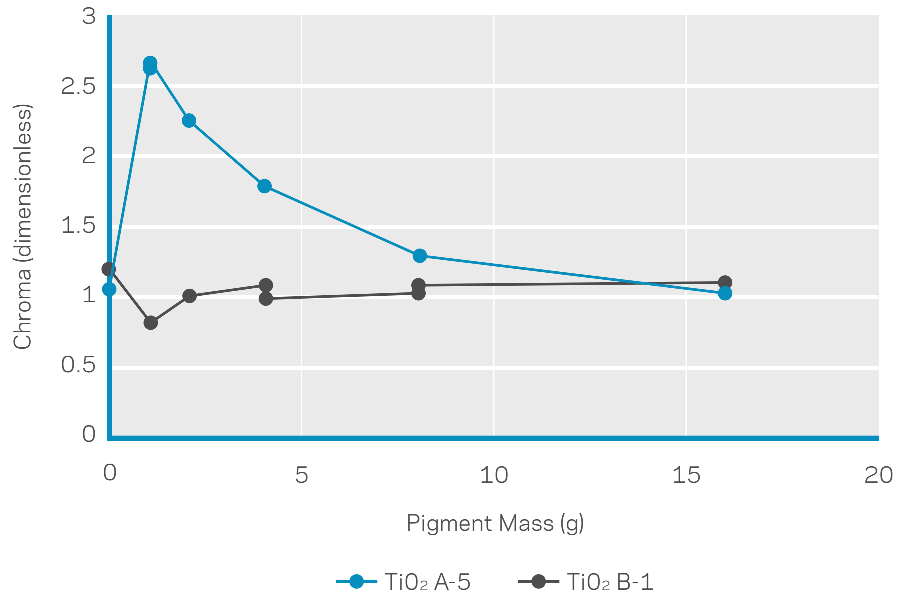


Figure 8. Effect of undertone and pigment concentration on the hue of samples (as measured by the difference in angle between the sample and standard as described in a polar coordinate system)

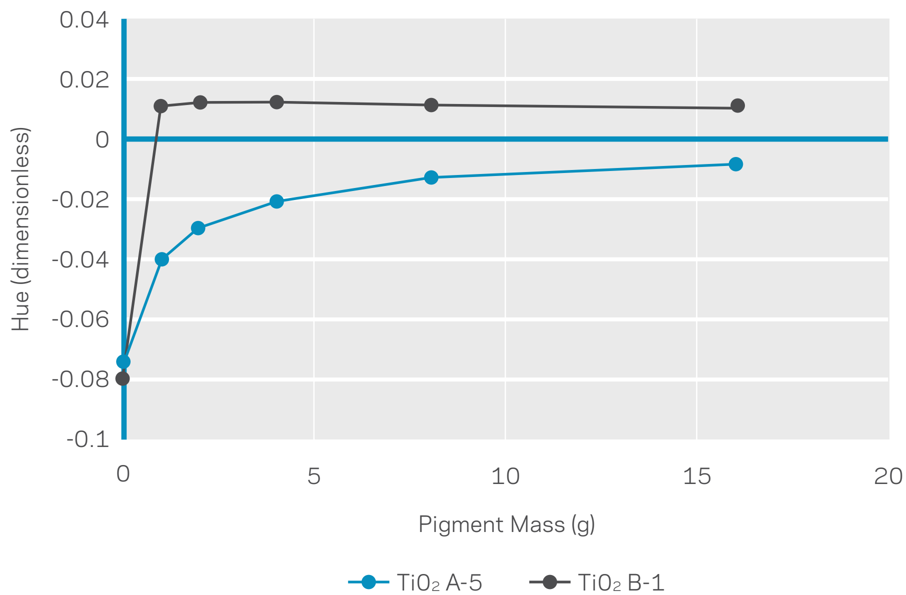
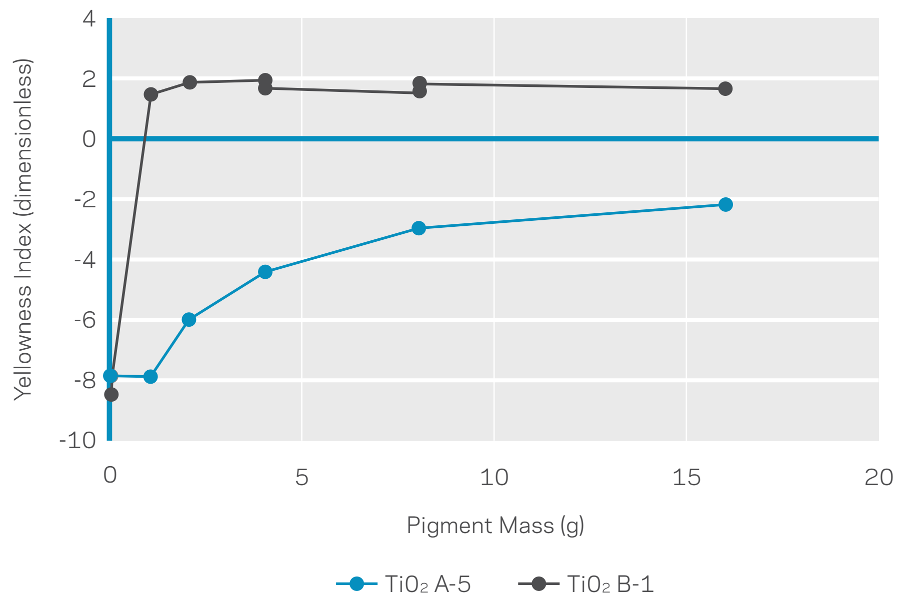


Figure 9. Effect of undertone and pigment concentration on the yellowness index of samples



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REFERENCES

Davis, S. P., Niedenzu, P. M., & Reid, A. H. (2010).
The Optical Impact of Low-Index Inorganic Fillers on the Performance of Plastic Articles Pigmented with Titanium Dioxide. Orlando, FL: ANTEC.

Feng, A. A., & Birmingham, J. N. (2003).
Use of Titanium Dioxide in Exterior PVC Applications. Wilmington, DE.

Horvath, H. (2009).
Gustav Mie and the scattering and absorption of light by particles: Historic developments and basics. *Quantitative Spectroscopy & Radiative Transfer,* 787-799.

Lilienfeld, P. (2004).
A Blue Sky History. *Optics and Photonics News,* 32-39.

Mie, G. (1908).
Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen. *Annalen der Physik,* 377-445.

Van de Hulst, H. (1981).
Light Scattering by Small Particles. New York: Dover Publications.

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