INTERNATIONAL STANDARD

ISO 18314-2

Second edition
2023-01

Analytical colorimetry —

Part 2: Saunderson correction, solutions of the Kubelka-Munk equation, tinting strength, depth of shade and hiding power

Analyse colorimétrique —

Partie 2: Correction de Saunderson, solutions de l'équation de Kubelka-Munk, pouvoir colorant, profondeur de teinte et pouvoir masquant

Reference number
ISO 18314-2:2023(E)

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Foreword

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This document was prepared by Technical Committee ISO/TC 256, *Pigments, dyestuffs and extenders,* in collaboration with the European Committee for Standardization (CEN) Technical Committee CEN/TC 298, *Pigments and extenders,* in accordance with the Agreement on technical cooperation between ISO and CEN (Vienna Agreement).

This second edition cancels and replaces the first edition (ISO 18314-2:2015), which has been technically revised.

The main changes are as follows:

— the title has been amended by “depth of shade”;

— the terms and definitions in Clause 3 have been aligned with ISO 18451-1;

— the document has been editorially revised and the bibliography has been updated.

A list of all parts in the ISO 18314 series can be found on the ISO website.

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Analytical colorimetry —

Part 2: Saunderson correction, solutions of the Kubelka-Munk equation, tinting strength, depth of shade and hiding power

1 Scope

This document specifies the Saunderson correction for different measurement geometries and the solutions of the Kubelka-Munk equation for hiding and transparent layers. It also specifies methods for the calculations of the tinting strength including the residual colour difference based on different criteria such as the depth of shade. Finally, methods for determining the hiding power are provided.

The procedures for preparing the samples for these measurements are not part of this document. They are agreed between the contracting parties or are described in other national or international standards.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

3.1
tinting strength
colour strength
measure of the ability of a colourant to colour other materials because of its absorptive power

[SOURCE: ISO 18451-1:2019, 3.122]

3.2
relative tinting strength
relative colour strength
percentage ratio of the *tinting strength* (3.1) of the colourant under test related to the tinting strength of a reference colourant

[SOURCE: ISO 18451-1:2019, 3.105]

3.3
tinting strength criterion
parameter that describes the colouring effect of a colourant, based on its absorption

Note 1 to entry: The tinting strength criteria used in this document are the following:

— value of the Kubelka-Munk function at the absorption maximum;

— weighted sum of the Kubelka-Munk function values;

— tristimulus value *Y*;

— the smallest of the tristimulus values *X*, *Y*, *Z*;

— shade depth parameter B.

Note 2 to entry: Examples of other tinting strength parameters not used in this document are the following:

— unweighted sum of the Kubelka-Munk function values;

— chromaticity given by the three colour coordinates (*L**, *a**, *b**);

— reflectance factor at the absorption maximum.

3.4
residual colour difference
colour difference that remains between the white reductions of the reference and test samples when the *tinting strength criterion* (3.3) values are the same or have been equalized

EXAMPLE Residual colour difference is given by ΔE^*.

3.5
depth of shade
shade depth
colour depth
measure for the intensity of a colour perception that increases with increasing chroma and decreases with increasing lightness

Note 1 to entry: Colourations having the same depth of shade appear to be prepared using the same concentrations of colourants having the same *tinting strength* (3.1).

[SOURCE: ISO 18451-1:2019, 3.26, modified — admitted terms "shade depth" and "colour depth" have been added.]

3.6
standard depth of shade
standard shade depth
standard colour depth
SD
depth of shade (3.5) level laid down by convention

[SOURCE: ISO 18451-1:2019, 3.113, modified — admitted terms "standard shade depth" and "standard colour depth" have been added.]

3.7
hiding power
ability of coating to obliterate the colour or colour differences of the substrate

Note 1 to entry: The use of the German expressions "Deckkraft" und "Deckfähigkeit" should be avoided.

Note 2 to entry: The term "coverage" is ambiguous because it is used in some instances to refer to hiding power and in others to mean spreading rate. The more precise terms hiding power and spreading rate should always be used.

[SOURCE: ISO 18451-1:2019, 3.47]

4 Symbols and abbreviated terms

a	constant
a^*	CIELAB colour coordinate
$a(\varphi)$	factor
$a(\lambda)$	auxiliary variable
b^*	CIELAB colour coordinate
$b(\lambda)$	auxiliary variable
B	shade depth parameter
C_{rel}	relative tinting strength
D_m	hiding power value indicating the area of the contrast substrate concerned, in m^2, which can be coated with 1 kg
D_v	hiding power value indicating the area of the contrast substrate concerned, in m^2, which can be coated with 1 l
$F(\lambda)$	Kubelka-Munk function
$F'(\lambda)$	modified Kubelka-Munk function
$g(\lambda)$	weighting function (defined as the sum of the colour matching functions $\bar{x}(\lambda)$, $\bar{y}(\lambda)$, and $\bar{z}(\lambda)$ for a 10° standard observer)
h	thickness
K	coefficient
$K(\lambda)$	absorption coefficient
$(K/S)_r$	Kubelka-Munk value of reference sample
$(K/S)_t$	Kubelka-Munk value of test sample
L^*	CIELAB lightness
m_r	mass fraction of coloured pigment reference sample
m_t	mass fraction of coloured pigment test sample
n	refractive index
r_0	reflection coefficient at the surface for directional light incident perpendicular from outside
$\overline{r_0}$	reflection coefficient at the surface for directional light incident parallel under 45° from outside
r_2	reflection coefficient for light incident diffusely from the inside of the specimen
$R(\lambda)$	reflectance spectrum
$R(\lambda)_\infty$	reflectance of infinitely thick layer
$R(\lambda)^*$	Saunderson-corrected reflectance spectrum

$R(\lambda)^*_{ob}$	Saunderson-corrected reflectance of the black substrate
$R(\lambda)^*_{ow}$	Saunderson-corrected reflectance of the white substrate
$R(\lambda)^*_{b}$	Saunderson-corrected reflectance of the sample on black substrate
$R(\lambda)^*_{w}$	Saunderson-corrected reflectance of the sample on white substrate
$R'(\lambda)$	modified reflectance spectrum including surface effects
s	saturation
$S(\lambda)$	scattering coefficient
SD	standard depth of shade
T	weighted sum
x, y	chromaticity coordinates
X, Y, Z	tristimulus values
ΔE^*	residual colour difference
ΔE^*_{ab}	CIELAB colour difference
φ	hue angle
φ_o	closest angle in the table below the hue angle
r	as a subscript, r refers to the reference sample
t	as a subscript, t refers to the test sample

5 Saunderson correction

5.1 General

For colorimetric calculation it is necessary to account for surface phenomena to obtain viable results. The formulae are known as Saunderson correction, and their derivation can be found in References [1] and [2]. The necessary coefficients are solutions of the Fresnel formulae[3] depending on the index of refraction for the given binder.

The formulae are derived assuming an ideal surface, a perfectly hiding layer and a perfectly diffuse scattering of light inside the interior of the specimen. Any deviation from these assumptions shall lead to consideration of the usefulness of the following calculations.

The formulae given here are for two of the most widespread geometries: diffuse incidence, 0° observation (d:0°) [Formula (1), Formula (2) and Formula (3)] and 45° incidence, 0° observation (45°:0°) [Formula (4) and Formula (5)]. In nearly every colorimeter used, the measurement angle is not 0° but 8°. This deviation is not considered problematic.

The constants necessary for the calculation are the following:

r_0 reflection coefficient at the surface for directional light incident perpendicular from outside. For $n = 1{,}5$ $r_0 = 0{,}040$.

$\overline{r_0}$ reflection coefficient at the surface for directional light incident parallel under 45° from outside. For n = 1,5, $\overline{r_0}$ = 0,050.

r_2 reflection coefficient for light incident diffusely from the inside of the specimen. For n = 1,5, r_2 = 0,596.

5.2 Incidence diffuse, observation 0° (d:0°)

The constant a = 1 if a gloss trap is closed and a = 0 if the gloss trap is open and the specular reflection is excluded.

$$R(\lambda) = ar_0 + \frac{(1-r_0)(1-r_2)R(\lambda)^*}{1-r_2R(\lambda)^*} \tag{1}$$

Where a = 1:

$$R(\lambda)^* = \frac{R(\lambda)-r_0}{1-r_0-r_2[1-R(\lambda)]} \tag{2}$$

Where a = 0:

$$R(\lambda)^* = \frac{R(\lambda)}{1-r_0-r_2+r_2[r_0+R(\lambda)]} \tag{3}$$

5.3 Incidence 45°, observation 0° (45°:0°)

$$R(\lambda) = \frac{(1-r_0)(1-\overline{r}_0)\frac{1}{n^2}R(\lambda)^*}{1-r_2R(\lambda)^*} \tag{4}$$

$$R(\lambda)^* = \frac{n^2R(\lambda)}{1-r_0-\overline{r}_0+r_0\overline{r}_0+n^2r_2R(\lambda)} \tag{5}$$

6 Solution of the Kubelka-Munk equations

6.1 General

The Kubelka-Munk theory describes the reflection of a pigmented layer by two constants: absorption, $K(\lambda)$, and scattering, $S(\lambda)$. It is based on the following assumptions:

a) ideally diffuse radiation distribution on the irradiation side;

b) ideally diffuse radiation distribution in the interior of the layer;

c) no consideration of surface phenomena resulting from the discontinuity in refractive index.

For an infinitely thick, respectively hiding layer with a reflectance of $R(\lambda)_\infty$, the following solutions shown in Formula (6) and Formula (7) are found, which allow the determination of the relation between the scattering and the absorption coefficient:

$$\frac{K(\lambda)}{S(\lambda)}=\frac{\left[1-R(\lambda)_\infty\right]^2}{2R(\lambda)_\infty}\equiv F\left[R(\lambda)_\infty\right] \tag{6}$$

respectively the inverse:

$$R(\lambda)_\infty=1+\frac{K(\lambda)}{S(\lambda)}-\sqrt{2\left[\frac{K(\lambda)}{S(\lambda)}\right]+\left[\frac{K(\lambda)}{S(\lambda)}\right]^2} \tag{7}$$

For the determination of the scattering and absorption coefficient, two different methods can be applied (the Saunderson correction shall be used).

6.2 Method 1

Measurement of the reflectance of an infinite thick (respectively hiding) layer and the reflectance $R(\lambda)^*$ of a coating of the thickness, h, on a substrate of the reflection $R(\lambda)_0^*$, then following Formulae (8), (9), (10), and (11):

$$a(\lambda)=\frac{1}{2}\left[\frac{1}{R(\lambda)_\infty^*}+R(\lambda)_\infty^*\right] \tag{8}$$

$$b(\lambda)=a(\lambda)-R(\lambda)_\infty^*=\frac{1}{2}\left[\frac{1}{R(\lambda)_\infty^*}-R(\lambda)_\infty^*\right] \tag{9}$$

$$S(\lambda)\ =\ \frac{1}{b(\lambda)\ h}\ \text{arcoth}\ \frac{1-a(\lambda)\left[R(\lambda)^*+R(\lambda)_0^*\right]+R(\lambda)^*\ R(\lambda)_0^*}{b(\lambda)\left[R(\lambda)^*-R(\lambda)_0^*\right]} \tag{10}$$

$$K(\lambda)=S(\lambda)[a(\lambda)-1] \tag{11}$$

6.3 Method 2

This method applies two layers of equal thickness, h, on black and white substances. After the determination of the auxiliary variables $a(\lambda)$ and $b(\lambda)$ according to Formula (12) and Formula (13), the scattering coefficient, $S(\lambda)$ can be calculated using Formula (14) or Formula (15). The possibility with the least experimental uncertainty should be chosen.

$$a(\lambda)=\frac{\left[1+R(\lambda)_\text{w}^*R(\lambda)_\text{ow}^*\right]\left[R(\lambda)_\text{b}^*-R(\lambda)_\text{ob}^*\right]+\left[1+R(\lambda)_\text{b}^*R(\lambda)_\text{ob}^*\right]\left[R(\lambda)_\text{ow}^*-R(\lambda)_\text{w}^*\right]}{2\left[R(\lambda)_\text{b}^*R(\lambda)_\text{ow}^*-R(\lambda)_\text{w}^*R(\lambda)_\text{ob}^*\right]} \tag{12}$$

$$b(\lambda)=\sqrt{a(\lambda)^2-1} \tag{13}$$

$$S(\lambda)=\frac{1}{b(\lambda)h}\text{arcoth}\frac{1-a(\lambda)\left[R(\lambda)_\text{b}^*+R(\lambda)_\text{ob}^*\right]+R(\lambda)_\text{b}^*R(\lambda)_\text{ob}^*}{b(\lambda)\left[R(\lambda)_\text{b}^*-R(\lambda)_\text{ob}^*\right]} \tag{14}$$

$$S(\lambda)=\frac{1}{b(\lambda)h}\operatorname{arcoth}\frac{1-a(\lambda)\left[R(\lambda)_{\mathrm{w}}^{*}+R(\lambda)_{\mathrm{ow}}^{*}\right]+R(\lambda)_{\mathrm{w}}^{*}R(\lambda)_{\mathrm{ow}}^{*}}{b(\lambda)\left[R(\lambda)_{\mathrm{w}}^{*}-R(\lambda)_{\mathrm{ow}}^{*}\right]} \tag{15}$$

Using $S(\lambda)$, the reflectance $R(\lambda)^*$ of a coating of the thickness, h, on a substrate of the reflection $R(\lambda)_0^*$ is given by Formula (16):

$$R(\lambda)^{*}=\frac{1-R(\lambda)_0^{*}\ \{a(\lambda)-b(\lambda)\coth[b(\lambda)\,S(\lambda)\,h]\}}{a(\lambda)-R(\lambda)_0^{*}+b(\lambda)\coth[b(\lambda)\,S(\lambda)\,h]} \tag{16}$$

NOTE The formulation of the Kubelka-Munk theory leads to a system of differential equations. The solution can be stated in different ways either by the use of the trigonometric functions used here or by the use of logarithmic functions. They are mathematically equivalent.

7 Determination of relative tinting strength and residual colour difference of coloured pigments

7.1 General

All the methods specified here presuppose, at least approximately, a linear relationship between the concentration of the colourant and the Kubelka-Munk function.

It is assumed that the scattering by the draw-downs being measured is dominated by the white pigment and the absorption by the coloured pigment. All these conditions shall be met to ascertain correct results of the methods described here. The Kubelka-Munk function for the white paste can be neglected in most cases.

7.2 Principle

The reference and test samples are incorporated into white pastes. The corresponding reflectance spectra are measured on opaque draw-downs of the resulting coloured pastes. The appropriate tinting strength criterion is calculated from the measured values.

If the tinting strength criterion values for the reference and test samples differ, the mass fraction of the sample is increased or decreased until the values become equal. This adjustment may be performed either experimentally or mathematically.

If the tinting strength criterion values for the reference and test samples are the same, or after they have been equalized, the residual colour difference between the white reductions of the reference and test samples is calculated from the corresponding reflectance spectra.

A spectrophotometer with d:8° or 8°:d measuring geometry with or without gloss trap, or instruments with 45°:0° or 0°:45° measuring geometry are recommended.

7.3 Procedure

7.3.1 General

The reflectance of an opaque draw-down of the white reduction of the reference sample and the corresponding reflectance of the test sample are measured in the visible spectral range.

7.3.2 Evaluation of absorption at the absorption maximum

The tinting strength criterion is the maximum Kubelka-Munk value. Prerequisite for this method are equal concentrations of reference and test pigments in the white pastes.