1ADVANCED COLOR FORMULATION

Color iMatch™

Doc-To-Help Standard Manual

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Contents

Abstract

Advanced Color Formulation

Traditionally, color formulation software has been based on theories whose mathematics cannot adequately address the complete needs of the color industry. The intention is to provide a solution that will address these needs and be a valuable tool for the beginner as well as the experienced colorist.

Unlike most commercially available color matching packages, solutions presented through the X-Rite® Color iMatch™ software are not based on Kubelka-Munk theory. All calculations are done in absolute units, and the same database can be used for matching samples that are opaque, transparent, or translucent. When used with a X-Rite Color i7™ or Color i5™ spectrophotometer, the same database can also be used to match samples in both reflectance and transmittance modes. Color iMatch flexibility means that a single package can be used for a wide variety of applications that include, but are not limited to: printing inks (offset, screen, gravure, and flexographic), coatings, and plastics. In addition to a new mathematical model, there are multiple features within Color iMatch that differentiate it from other color matching packages.

Due to the proprietary nature of the mathematics used in Color iMatch, not all features will be covered in complete detail.

Traditional Color Matching

Visual Color Evaluation

Color matching is still as much an art as it is a science, and the importance of visual evaluation must not be taken for granted. There still is no substitute for the visual evaluation of color, though it is used more in the quality control function and less in the determination of initial formulas.

Traditionally initial matches required significant trial and error, even with a highly skilled color matcher. In most organizations the color matcher is aided by instrumental and computational methods to supplement visual evaluation. Besides more accurate formulations, the most important advantage to the use of a computer formulation system is the amount of time that it takes to obtain an initial match. By significantly decreasing the amount of time it takes to obtain an acceptable match the profitability of the end product can increase dramatically.

Visual Evaluation Requirements

For successful visual evaluation of color, there are three important criteria that must be met. The most important requirement is normal color vision. However, the cases where thorough color vision testing is employed are far and few between. By using a test method such as the Farnsworth-Munsell 100 Hue Test, the level of color deficiency can easily be determined. A controlled viewing environment, with standard light sources like the X-Rite SpectraLight® III, is also an important part of visual evaluation. Finally, there is no substitute for experience. Today it is becoming more difficult to find sufficiently experienced personnel. Instrumental methods help to reduce the amount of experience required and decrease the learning curve when developing visual evaluation skills.

Additivity Principle

The additivity principle means that if two pigments are mixed in a sample, the total absorption can be found by adding up the individual absorption's of the pigments. Both pigments behave as if the other one was not there. An example of this behavior is described in the following equation using K/S.

(K/S)a+b = (K/S)a + (K/S)b

Experimental data has shown that the additivity principle is not generally valid for a mix of two or more pigments.[4]

K/S *versus* Wavelength

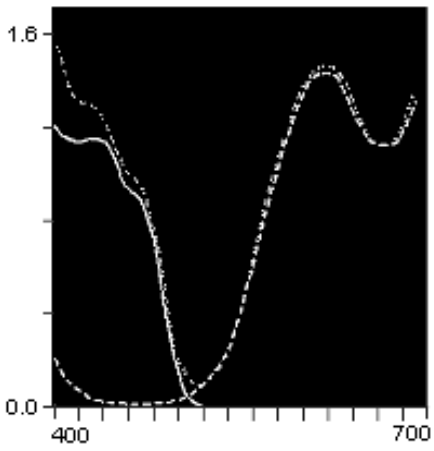

Figure 1a

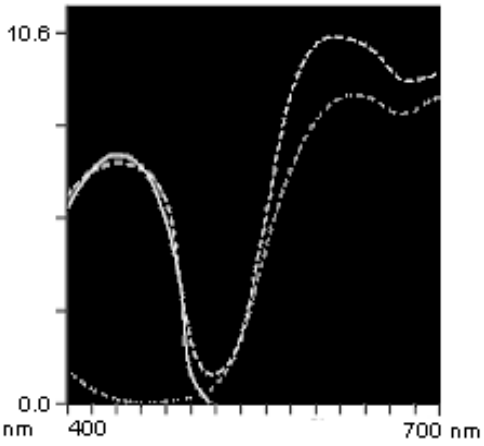

Figure 1b

In Figure 1a it can be seen that the additivity theory is valid in some cases; but it does not always hold true, as can be seen in Figure 1b.

Kubelka-Munk

The Kubelka-Munk theory is used for reflectance measurements and calculations. The original Kubelka-Munk theory described the propagation of light in a stellar system. The same equations have been used for the interaction of light with pigment particles in paint, plastic, and ink mediums. Although these applications are considering the same visible light; the distance between, and the dimensions of, pigment particles versus those of the stars are quite different.[4]

Originally published in the1930's by Paul Kubelka and Franz Munk, the Kubelka-Munk equations described the reflectance and transmittance of the sample as a function of absorption and scatter (K and S respectively). The Kubelka-Munk theory is a two-flux version of the many-flux method of solving radiation transfer problems.[6] Given that the sample must have the same refractive index as air these equations were not practical for industrial color matching. In the 1940's the Saunderson correction factors were introduced and the Kubelka-Munk equations became more practical for the use in opaque systems. Simplifications and assumptions have been made to the original equations, though these simplified formulas have many limitations they are the dominant algorithms used in color matching systems today.

Single and Two Constant

Depending on the application, the Kubelka-Munk equations can be divided into two different cases; single constant systems and two constant systems.

Single Constant

Single constant theory assumes that the individual pigments do not significantly contribute to the total scattering of the sample. An example of this theory is the exhausting of transparent dyes into a textile substrate.

Two Constant

If the scatter is assumed to occur from two sources, the colorant(s) and the substrate, it is considered two constant theory. An example of this theory is the formulation of opaque coatings where titanium dioxide is blended with other pigments to achieve color. In this case the titanium dioxide becomes the second source of scatter.

Saunderson Correction

Given the limitations of Kubelka-Munk a more complex equation was developed by J.L. Saunderson that contrasted the refractive index of the sample to that of air. With the addition of surface or specular (K1) and internal (K2) correction factors the equation became more practical for use in opaque systems.

Deficiencies of Kubelka-Munk Theory

Though the Kubelka-Munk theory has proven to be adequate in many applications it has significant deficiencies that prevent it from being a total solution for color matching. Kubelka-Munk theory continues to be popular because it provides simple analytical equations and reasonable predictions.[6]

Assumptions of Kubelka-Munk

It is assumed that the colorant layer is sufficient in extent for there to be no light lost from the edges of the layer and that it has uniform composition.[6]

Kubelka-Munk reflectances arise from the assumption that the coefficients K and S are the same for forward and reverse flux. From a many-flux analysis it can be concluded that the angular distribution of the forward and reverse flux is not the same.[6]

The Kubelka-Munk theory assumes a linear relation between the colorant characteristic K/S and the colorant concentration. In general it is found that the K/S ratio of a component colorant is a nonlinear function of the concentration.[7] This means that it will not be possible to adequately describe the colorant behavior by using a linear relation.

K/S *versus* Concentration

420 nm

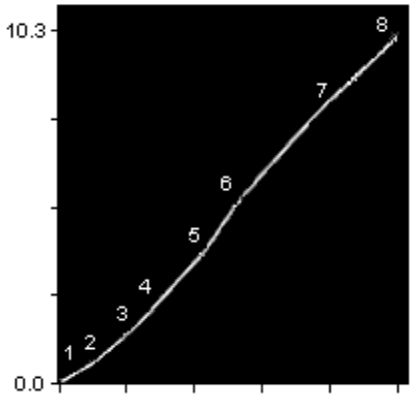

Figure 2a

520 nm

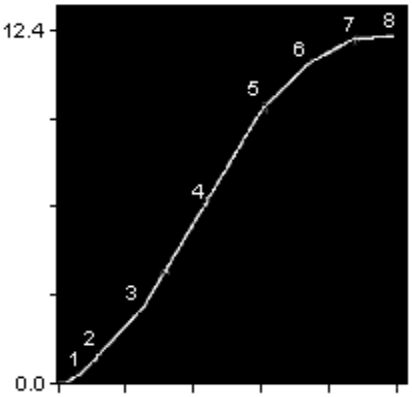

Figure 2b

Figure 2a shows the linear relation that results between K/S and concentration. In figure 2b the plot shows a typical non-linear relationship between K/S and concentration at 520 nanometers for a series of calibration samples.

For the Kubelka-Munk theory to work it is assumed that the pigment particles act independently of each other. The net result is obtained simply by adding up the individual actions.[4]

Lambert-Beer

The Lambert-Beer theory is reserved for transmittance calculations for very transparent samples. Dating back to the 18th and 19th centuries, the Lambert-Beer law states that the absorbence (Log 1/*T*) for a transparent sample is proportional to the thickness and the concentration of the colorant.[1]

Beer's law has been found to be valid at low and moderate concentrations in transparent applications but it may prove to be inaccurate at higher concentrations. In order for Beer's law to be valid the absorption coefficient must be a constant independent of the concentration.[3] Since all colorant layers scatter some light; these equations, even in cases of slightly turbid-media, are generally not valid.

Advanced Color Matching

Turbid-Medium Theory

Though Kubelka-Munk is a turbid-medium theory, it is limited in its application. It is important to note the advancements that have been made in other areas of turbid-media theory. This will help to determine which will best accommodate the different types of samples we see in today's color industry.

Turbid-Media

There are three kinds of optical systems that define turbid-media; optically thin, intermediate, and optically thick. Each of these systems can be seen throughout our everyday lives and each one is significantly different from the other. Of all the theories that have been developed to handle the turbid-mediums, only one can successfully handle all three optical systems.

Optically Thin

The scattered light that is observed is scattered only once; much unscattered light emerges from the sample.[2] An example of an optically thin application would be transparent *dyes* being exhausted into a textile substrate.

Intermediate

Most of the scattered light has been scattered many times, but some unscattered light emerges from the sample.[2] A typical intermediate application would be a plastics operation that works with pigments and general purpose polystyrene. Most systems that are typically assumed to fall into the optically thin and optically thick areas are actually intermediate media. Classically, offset printing inks are assumed to be optically thin and screen printing inks to be optically thick. In most cases both of these applications fall into the intermediate media classification.

Optically Thick

All the light has been multiply scattered.[2] A paint manufacturer preparing opaque coatings, where titanium dioxide is blended with other scattering pigments to create a color, would be considered an optically thick system.

Application of Turbid-Medium Theories[2]

Theory	Optically Thin	Intermediate	Optically Thick
Kubelka-Munk	No	No	Yes
Four-Flux	Yes	Limited	Yes
Many-Flux	**Yes**	**Yes**	**Yes**
Doubling	Yes	Yes	Limited
Monte Carlo	Yes	Limited	No
Scattering Order	Yes	Limited	No
Diffusion	No	No	Yes

Billmeyer and Richards examined various turbid-medium theories for their applicability in the three levels of optical behavior.[2] Of all the theories shown only the Many-Flux method accommodates all three turbid-media classifications.

Many-Flux

The many-flux theory covers applications with all levels of optical thickness from one mathematical model. By using this model to determine absolute K and S values, the software does not have to define whether white is present in the formulation. All matching is done in one database. There is no need for separate packages that would use Kubelka-Munk single constant, Kubelka-Munk two constant or Lambert-Beer mathematics.

Color iMatch System

Color iMatch

Color iMatch is a sophisticated and intuitive color formulation and quality control tool that is easily learned and used by the expert as well as the novice color matcher.

Color iMatch automatically determines the best formula for your application based on the parameters you select, such as lowest cost or least number of colorants. It will automatically formulate with or without white, at all levels of opacity, from a single database. In addition Color iMatch Satellite Systems can offer added value by providing the same high quality formulation results as a full Color iMatch system, with a low cost and feature limited satellite.

With the continuing advancement of the personal computer, more complicated calculations can be done in less time.

These advancements in personal computers have given Color iMatch the ability to perform many complicated algorithms, such as computing many-flux calculations and spectral matching routines.

Kubelka-Munk Comparison with Color iMatch

Color iMatch is *not* based on Kubelka-Munk

Two Constant Always Used

Although a number of colorants can have very low absorption (extenders, resins, etc.) or a very low scattering (several pigments, colorants, etc.), there is no such thing as zero absorption or zero scattering. There is no single constant behavior in the real world, nature is always two constant. Because all samples show two constant behavior, the calculations in are based on two constant mathematics.[4] Though Kubelka-Munk used two-constant theory in some cases, it is limited due to the simplified equations and the assumptions about sample and colorant characteristics.

All Calculations in Absolute Units

K and S[4]

Due to the mathematical restrictions of the Kubelka-Munk equations, the pigment K and S data are calculated relative to a reference component (generally the white pigment). Typically the K and S of the white can be determined with a double measurement (reflectance and transmittance or over white and over black). This is performed on an individual sample or series of samples at constant thickness and varying white pigment volume concentrations. This does allow for the optimization of white pigment loading, though it can result in inaccurate calculations of opacity and/or pigment loading when considered in combination with other colorants.

From the beginning Color iMatch calculates pigment K and S in absolute units. In addition the calculation of K and S goes beyond the white pigment to *all colorants* providing accurate opacity and pigment loading predictions.

K and S *versus* Wavelength

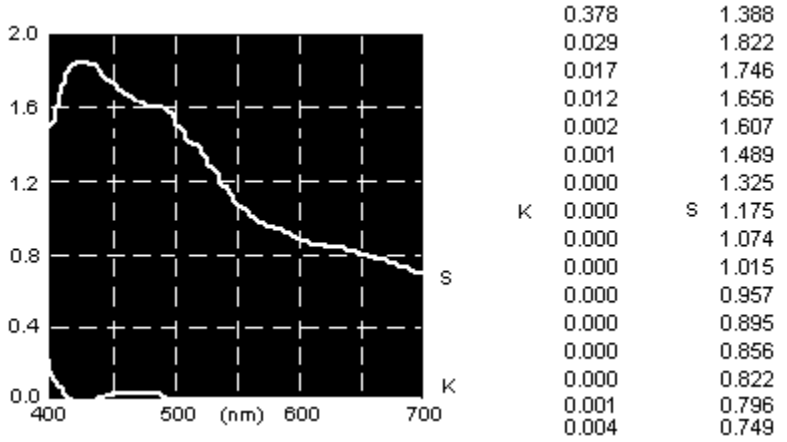

Figure 3

The data in figure 3 shows calculated K and S data, where both K and S are variable across the visible spectrum.

K1 and K2

The Kubelka-Munk equation is founded on the premise that once you disperse a pigment in a resin system, there is no further development. The determination of how much light enters a sample and how much exits after diffusion, relates directly to the Saunderson correction factors, K1 and K2.[5] However, most available software uses a fixed value for K1 and/or K2. In many cases these values are not calculated, they are input by the user. For example, default values of 4% for K1 and 60% for K2. These values are fixed for all wavelengths or they can be a calculated value limited to a single wavelength. These methods are not valid because K1 and K2 are dependent on the refractive index of the material which is wavelength dependent (see figure 4). Depending on the sample set, using a fixed K1, K2 value can lead to inaccurate calculation of absolute K and S. Color iMatch calculates and takes advantage of K1 and K2 values at each wavelength.

K1 and K2 *versus* Wavelength

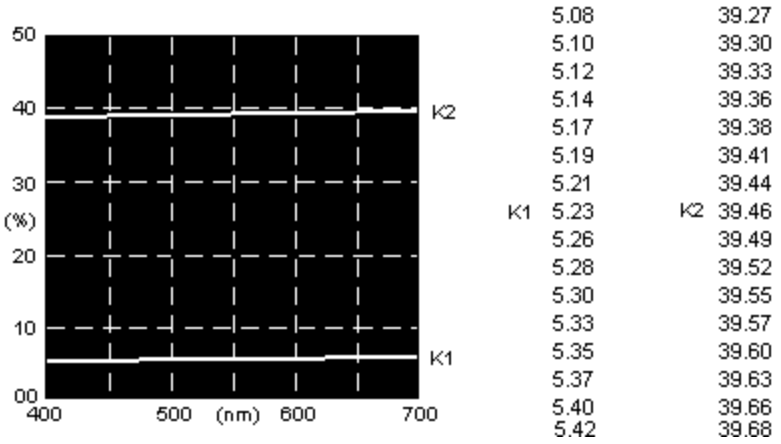

Figure 4

Figure 4 shows the variation that can occur in the determination of the K1 and K2 values at individual wavelengths across the spectrum.

As colorants are added to a Color iMatch database the K1 and K2 values will change. This implies that other samples added to the database can influence the K1 and K2 values. This occurs because the added samples will give better characterization. The system can then calculate more accurate values. In many cases other formulation packages will base its K1 and K2 calculations solely on the resin, white and black.

Non-Linear Relationships

Kubelka-Munk assumes linear relationships for K/S versus concentration and K/S versus thickness as well as the validity of the additive theory.

1. K (Concentration)
2. S (Concentration)
3. K (Thickness)
4. S (Thickness)
5. "Additivity"

Color iMatch treats all functions as completely non-linear; it does not try to approach non-linear functions through a piece by piece linear approximation.

Calibration Uses All Selected Samples

Because Color iMatch works from a single database, all selected samples are used in the calibration process. Calibration samples can consist of opaque, translucent, and transparent samples as well as samples at multiple film thicknesses. Measurements can be reflectance only, reflectance and transmittance, over white and over black, or any combination of these measurements.

Additivity Principle Not Used

Color iMatch uses a non-linear function for the relationship between both K and S and the pigment concentration. When two or more pigments are mixed into a sample, an interaction is calculated.[4]

Many-Flux

The many-flux theory can be applied to applications that have samples at any level of optical thickness. All the calculations can be done in a single formulation package.

Two-Flux *versus* Many-Flux

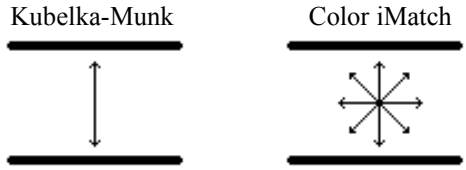

Figure 5

The physics that takes place within the colorant/resin matrix demands that directional flux be determined. Color iMatch considers light flux within the colorant/resin matrix in both an up and down flux (Kubelka-Munk) as well as directional flux.

Spectral *versus* Tristimulus Matching

Tristimulus Match

The typical approach for color formulation uses tristimulus matching routines.

Match Routine

Match standard X, Y, Z
Three equations to be solved
3 Unknowns = 3 Concentrations = 3 Pigments

Disadvantages

Because there are three unknowns there needs to be at least three pigments in the formula.

2 Pigments: impossible

1 Pigment: impossible

Spectral Match -- Color iMatch

In Color iMatch the computations are completed through an iteration process. There is no exact tristimulus match, but a best fit spectral curve match is calculated. This is not a selective spectral match; all Color iMatch formulations are done using its spectral matching routine.

Match Routine

Match standard spectral data R_i
Iteration to achieve best fit

Advantages

1. Better pigment selection due to more points of reference.
2. No limitation on the number of pigments (minimum or maximum)
3. Metamerism is minimized in calculations (spectral matching ensures quality under all lighting conditions, not just default conditions)
4. More accurate formulations in general.

Dynamic Database

Color iMatch has the capability to continually add more samples to the calibration database in order to increase performance. In addition, the sample set is variable for each individual colorant. An application may require only five samples for a yellow colorant, but twelve samples for a reflex blue to achieve optimum performance. Note that additional samples, including mixtures of multiple colorants, are used in the calculation of the absolute K and S data. These samples are *not* a function in a "search and correct" calculation.

Complete file calibration uses all selected samples and optimizes the K and S data for all colorants. The results for *all* matches will improve, not just matches that are close in color or formula to the added samples.

Sample Set

In some cases the sample set may appear to be more extensive than what is requested for other formulation packages. However the amount of work and time involved may actually be less. If a typical sample set requires two individual samples at opacity and each sample must be cross-coated five times to reach opacity, the number of drawdowns that must be made is ten (with time to dry between each cross-coat). If Color iMatch requires eight individual samples there are only eight drawdowns at process thickness, with no drying time in between.

Samples for Color iMatch Database

1. Mathematical Minimum: 2
   (2 unknowns --- 2 knowns)
   Linear relation is always correct (straight line, one sample)
   Sample validity can not be determined
   Concentration dependent
2. Non-Linear Relation (More Than Two Samples)
   samples that are not correct can be easily identified.
   More samples, better characterization
3. Types of Samples for Each Colorant
   Different concentrations with resin
   Mixes with white (help to define white using “non gray” samples)
   Mixes with black (lower reflectance values help to define K1)
4. Number of Samples
   Application dependent
   Typically 7-10 samples per colorant
5. Additional Samples
   Once the database is complete it is possible to add more calibration samples to improve performance if necessary.
   All that is required the measuring of the new sample(s) and re-calibrating the database.
6. Known Mixtures
   Mixtures of multiple colorants may also be used to characterize the database.

Sample Characteristics

In many Kubelka-Munk based color matching systems the user is required to present an opaque sample to the spectrophotometer. Depending on the application this can be done a number of ways. For coatings the technique of cross-coating several layers of colorant until opacity is achieved is commonly used. The generated sample then has become inconsistent with the typical process thickness. Although this can add error to the formulation it will still adhere to the limitations of the Kubelka-Munk equation. [5]

The samples required for the Color iMatch system must be at process thickness for the most accurate characterization of each colorant. Unlike Kubelka-Munk samples, Color iMatch can benefit from samples that have not reached complete opacity. The sample’s colorant thickness is also used in the calibration process. This enables the user to enter the same sample at different thicknesses into the database. This is important for applications that continually produce samples at varying film thicknesses.

Effect of Sample Set

Full *versus* Limited Sample Set

		Resin	White	Black	Yellow	Red	Green	Blue
1.	Actual	90	300	30	60	0	60	60
	Full	90	302	37	61	0	67	46
	Limited	90	301	0	77	24	40	69
2.	Actual	60	120	120	0	60	0	240
	Full	60	118	125	0	53	0	244
	Limited	60	106	155	0	13	0	266
3.	Actual	120	0	0	180	240	0	60
	Full	120	1	0	192	242	0	45
	Limited	120	0	82	199	197	2	0
4.	Actual	300	30	30	0	180	60	0
	Full	300	27	33	0	189	52	0
	Limited	300	25	39	27	168	442	0

Figure 6

Figure 6 shows how the number of samples used to characterize a database can affect the initial formulation. In this example the full set uses nine samples (six masstone letdowns, one with white, one with black, and one with white and black) per colorant and the limited uses three samples (one masstone, one with white, and one with black). The nine sample database provides initial predictions that are much closer to the actual formula.

Applications

Because basic pigment properties are calculated using absolute units, how they are applied in the matching algorithm add versatility to the Color iMatch system

Single Database

The same database can be used for samples at all levels of opacity; transparent, translucent, and opaque. The quality of the predicted recipes will be the same for all degrees of opacity.

Multiple Mediums

It is not necessary to characterize the pigment behavior in all mediums. Multiple resin systems (different bases, extenders, clears, etc.) can be calibrated into one database. This process only requires samples mixed with white and black for each additional resin that is added.

Reflectance and Transmission

Both reflectance and transmittance measurements can be applied to the same database. For plastics, translucent liquids, and for printing or coating on non-opaque substrates this is a very important feature. In these applications it is not sufficient to match a standard in reflectance only, a transmission match is equally important. Color iMatch can combine both types of matches in one calculation, using only one database. In order to use this capability it is necessary that the spectrophotometer can

measure both the reflectance and total transmission of the sample (i.e., X-Rite Color-Eye 7000).

Contrast Measurements

Just as the reflectance and transmittance measurements can be used in one database, contrast measurements can also be applied to a single database (or even combined with R/T measurements for the calibration of the database). In this case the two measurements that would be combined are the over white and over black measurements. Typically this technique is applied to coatings and printing inks on paper or screen inks on textiles (white and black cloth).

Summary

Advanced Color Formulation

In practice there are many sources of error apart from the inaccuracies of theory. In addition there is human error, measurement error, batch variation of the colorants, and the non-reproducibility of the coloration process itself.[6] Once a process is under control, the next step is to apply color formulation software. It has been shown that many of the past methods have not proven to be completely viable for the variety of color applications that we encounter today.

The solutions presented through the X-Rite Color iMatch software are not based on Kubelka-Munk theory. All calculations are done in absolute units, and the same database can be used for matching samples that are opaque, transparent, or translucent. The database can be calibrated using samples measured in reflectance, reflectance and transmittance, or contrast modes. Color iMatch uses a single mathematical model that can be used for a wide variety of applications. There are many features within Color iMatch that can differentiate it from other color matching packages.

Considering the full scope of many applications, other commercially available packages have not been able to provide a total solution for color matching. With the addition of the many-flux theory, variable K1 and K2 values, and spectral matching Color iMatch is the next step in providing the color industry with a *total* solution for color formulation.

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