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Reflectance and transmittance of flowable dental resin composite predicted by the two-flux model: on the importance of analyzing the effective measurement geometry

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Abstract

Flowable direct resin composite materials used in the dental domain are among materials that scatter light rather weakly, giving to millimeter-thick samples a certain translucent aspect. In order to predict the spectral reflectance and the color of such samples, the two-flux theory, i.e., Kubelka-Munk model (with Saunderson correction), remains the standard approach used in the dental domain, in spite of its known limitations when scattering is too weak. The present study, however, shows that a careful analysis of the light signal effectively measured on weakly scattering samples with instruments based, as usually recommended, on the d:8° measurement geometry, and a subsequent reevaluation of the parameters used in the Saunderson correction formulas with respect to the effective measurement geometry, can considerably improve the prediction accuracy of the model in both reflectance and transmittance modes, as confirmed by experiments carried out with samples of dental flowable resin composite material of different thicknesses. This broadens the applicability domain of the model, and might satisfy users preferring the simplicity of the two-flux model and the affordable equipment it needs to more relevant but more complex light scattering theories.

1. Introduction

Because of its simplicity, its close-form formulas, and the reduced number of measurements needed for calibration, the Kubelka-Munk model [1-3] remains the favorite approach in many application domains to predict the color of a diffusing material, or the color change of a backing on which this material is coated, through the prediction of the spectral reflectance of the material layer according to its thickness. It is widely used for example in the dental domain for color prediction or color formulation of dental composite materials, the kind of materials that will be considered here. However, the simplicity of the model relies on restrictive assumptions regarding the description of light propagation within the material. The model is well adapted to strongly scattering media [4], or, more precisely, to layers of scattering medium thick enough to give rise to an intense multiple light scattering process. However, it is more problematic in cases of weak scattering, for different reasons widely discussed in the literature, in particular through comparative analyses of the light transfers at infinitesimal scale as described by the Kubelka-Munk model and by the radiative transfer theory (see for example Ref. [5]). The measuring geometry for the reflectance and transmittance measurements, although less investigated, is also an important factor of the predictive performance, as we will show in this paper.

The Kubelka-Munk model assumes that the incident light is perfectly diffused and that all the exiting light is accounted for in the measurement [6], which corresponds to a bi-hemispherical reflectance as defined by Nicodemus [7]. However, this geometry remains ideal and is not available in practice. In the case of strongly scattering layers, a hemispherical-directional geometry (e.g., the d:8° geometry recommended by the CIE [8]) or a directional-hemispherical geometry (e.g., 0°:d geometry) are good alternatives, as they are equivalent in this case to the bi-hemispherical geometry from a radiometric point of view. But this is not true for weakly scattering layers: a collimated illumination or detection implies that part of the flux captured has followed a rather straightforward path from the source to the detector, and is not representative of the diffuse light transfers described by the model. Significant error can arise if the geometry is not carefully taken into account in the equations, especially the ones describing the reflections and transmissions of light at the air-material interface with respect to the angular distribution of light (so-called Saunderson correction [9]). Formulas adapted to a directional-hemispherical geometry have been proposed for a layer of material coated on backings [10], as the method relying on white and black backings is the most common method, in particular in the dental materials domain, to derive the absorption and scattering coefficients [11-16]. However, for the alternative calibration method based on reflectance and transmittance measurements considered here, the radiometric consideration of the angular distribution of light at the interfaces has not been done so far, although it is crucial, as we show, for a good predictive performance.

Translucency of the material causes another, purely practical problem for reflectance/transmittance measurement: the wide point spread function characteristic of every translucent material [17-19] causes a "light-loss" in reflectance or transmittance measurements, comparable to the well-known "red-loss" phenomenon often observed with human skin [20], which distorts the spectra measured, usually underestimated.

These two points related to reflectance/transmittance measurement issues will be explicitly addressed in this paper, and the two-flux model will be revised accordingly. Prior to the revision in Section 3, the classical two-flux model and the computation of the absorption and scattering coefficients from measured reflectance and transmittance factors are recalled as usually presented, and generally adapted to strongly scattering media. The model itself is recalled in Section 2, as well as the

computation of the absorption and scattering coefficients from the measured reflectance and transmittance. Then, in Section 4, measurement issues are addressed and corrections of the model's parameters, especially for the flux transfers at the interfaces, are presented. An experimental verification, carried out on translucent dental composite materials, is proposed in Section 5. Section 6 finally draws the conclusions.

2. The classical two-flux model

The two-flux reflectance and transmittance prediction model predicting for slices of light scattering material relies on two models: the Kubelka-Munk model [1,2] describing the light flux propagation through the bulk material itself, and the so-called Saunderson correction [9] describing the reflections and transmissions of light at its interfaces with air. The material's optical properties are characterized by three parameters: optical index, spectral absorption coefficient $K(\lambda)$, and spectral scattering coefficient $S(\lambda)$. After a necessary comment on the reflectance and transmittance concepts, we propose to recall the main results of the two-flux model by highlighting its assumptions.

On reflectance and transmittance

Strongly scattering layers have an interesting radiometric property: independently of the illumination geometry (directional or diffuse), the light reflected is perfectly diffused, and more precisely the radiance reemitted by the medium is the same in every direction of the hemisphere. A layer presenting this property is said to be a Lambertian reflector. However, a diffusing medium, even a very diffusing one, having a smooth interface with air does not satisfy this property: the reflections and transmissions of light by the interface are angle-dependent and modify the angular distribution of the light entering and exiting the medium. In this context, it is important to take rigorously into account the geometry of illumination and light collection in the analysis of the measured quantities.

Let us insist on the difference between *reflectance*, ratio of reflected to incident fluxes, and *reflectance factor*, ratio of the light quantity measured on the considered sample to the light quantity measured on a perfectly white diffuser with reflectance close to 1 [7]. Reflectance factor is actually the quantity measured by most reflectance measuring instruments; it coincides exactly with reflectance in the case of Lambertian reflectors, and only in this case. Thus, the two concepts differ from each other in the case of scattering materials with smooth interface with air, according to the explanations above. Same considerations apply with light transmission, for which is defined the *transmittance* (ratio of transmitted to incident fluxes) and *transmittance factor* (ratio of measured light quantity through the sample, to measured light quantity in absence of sample).

For both reflectance/transmittance and reflectance/transmittance factor concepts, the measuring geometry, i.e. the angular distribution of the incident light and the direction(s) from which light is collected, must be explicitly specified. In the context of the Kubelka-Munk model, as the incident light is assumed to be perfectly diffused, an integrating sphere is often used for illumination (so-called hemispherical illumination [7]). As the integrating sphere cannot be used for both illumination and collection of the reflected/transmitted light, this latter is often collected in one direction (e.g., at 8° from the normal of the surface, as recommended by the CIE, which corresponds to the geometry denoted as d:8° [8]). For a strongly scattering surface, i.e., a Lambertian reflector, collecting the whole reflected exitance or only the radiance reflected in one direction is equivalent: according to Lambert's law [22], exitance and radiance in any direction are proportional to each other (i.e., related by a factor π, which cancels when computing the reflectance factor since same factor applies to the reflector and the perfectly white diffuser). However, in the opposite case where the medium is non scattering, e.g., a mirror in reflectance mode, or a tile of transparent medium in transmission mode, even though the integrating sphere provides diffuse light, only the incident light ray incoming at 8° can be captured by the detection system, and the effective measuring geometry is 8°:8°, as explained in [23]. This is crucial to have this in mind when analyzing the measured quantities and using them in a prediction model for this kind of materials.

In the intermediate case of a weakly scattering medium, the effective measurement geometry is not precisely known. It is certain that the light captured by the detector does not originate from the whole hemisphere, but rather from a certain "cone" around the incidence direction at 8° from the normal of the sample, which leads us to distinguish the *instrument geometry* (e.g., d:8° hemispherical-directional geometry) from the *effective measurement geometry* (e.g., conical-directional geometry). This will be one of the points discussed in Section 3. But let us now remind the Kubelka-Munk model in the case where its validity is recognized, i.e., in the case of strongly scattering media.

Kubelka-Munk model

The Kubelka-Munk model describes light propagation in a layer of scattering medium considered without any interface at its boundaries, as if the medium was surrounded by a clear medium with same optical index. A system of two differential equations represents the attenuation due to absorption, and mutual exchanges due to backscattering, of two fluxes assumed perfectly diffused going into opposite directions. The model requires a perfectly diffuse, i.e., Lambertian, irradiance.

The "intrinsic" reflectance ρ_h and transmittance τ_h of a layer of medium with thickness h, the term "intrinsic" reminding that the medium is considered without interfaces at its boundaries, are given by close form formulas issued from integration of the differential equation system:

$$\rho_h = \frac{\sinh(bSh)}{b\cosh(bSh) + a\sinh(bSh)} \tag{1}$$

and

$$\tau_h = \frac{b}{b\cosh(bSh) + a\sinh(bSh)} \tag{2}$$

where K and S denote the absorption and scattering coefficients, respectively, and

$$a = (K+S)/S \quad \text{and} \quad b = \sqrt{a^2 - 1} \tag{3}$$

Notice that parameter a can also be expressed as a function of the intrinsic reflectance and transmittance of a layer of any thickness:

$$a = \frac{1 + \rho_h^2 - \tau_h^2}{2\rho_h} \tag{4}$$

All parameters here, except the thickness *h*, may depend upon wavelength of light.

Saunderson correction

In order to account for flux transfers at the interfaces bordering the layer, by assuming that same clear medium surrounds the two faces of the layer (e.g., air, with a refractive index close to 1), the following formulas give the relationship between the reflectance and transmittance factors, *R* and *T*, which can be measured with an instrument and the intrinsic reflectance and transmittance of the medium itself, ρ and τ, which cannot be measured directly:

$$R = r_e + T_{in}T_{out}\frac{\rho - r_i\left(\rho^2 - \tau^2\right)}{\left(1 - r_i\rho\right)^2 - r_i^2\tau^2} \tag{5}$$

and

$$T = \frac{T'_{in}T'_{out}\tau}{\left(1 - r_i\rho\right)^2 - r_i^2\tau^2} \tag{6}$$

where the terms r_e, r_i, T_{in}, T'_{in}, T_{out} and T'_{out} denote flux transfers at the interface, detailed below by assuming that the interface is smooth. They all depend on the optical index of the medium, and are derived from the Fresnel formulae with respect to the illumination and observation geometries. In this paper, we consider the hemispherical-directional d:8° geometry where the incident light is Lambertian and only the radiance at 8° from the normal of the sample is captured. Their respective expressions and values for other measuring geometries, in particular the 45°:0° geometry, are detailed in [24]. We consider that same geometry is used for reflectance and transmittance measurement, therefore that $T_{in} = T'_{in}$ and $T_{out} = T'_{out}$. As in Ref. [23], the Fresnel reflectance is denoted as $R_{12}(\theta)$, resp. $R_{21}(\theta)$, when the incidence angle is θ at the air side, resp. the medium side.

r_e represents the fraction of light, if any, being specularly reflected from the source to the detector. It is either $r_e = R_{12}(8°)$ if the specular reflection component is included, or $r_e = 0$ if it is excluded, the two options being often proposed by measuring instruments.

r_i represents the fraction of diffuse light, assumed to be Lambertian, that is reflected by the interface at the medium side ("internal reflection"). It is obtained by integrating the angular Fresnel reflectance $R_{21}(\theta)$ in the following way (tabulated values according to the refractive index have been proposed by Judd [25], and can also be found in Ref. [23]):

$$r_i = \int_{\theta=0}^{\pi/2} R_{21}(\theta)\sin 2\theta d\theta \tag{7}$$

T_{in} represents the fraction of diffuse incident light crossing the interface from air to medium, according to the geometry. With a d:8° geometry, it is obtained by integrating the angular transmittance $T_{12}(\theta) = 1 - R_{12}(\theta)$ over the hemisphere:

$$T_{in} = \int_{\theta=0}^{\pi/2} T_{12}(\theta)\sin 2\theta d\theta = n^2(1 - r_i) \tag{8}$$

Finally, T_{out} represents the fraction of radiance issued from the medium that crosses the interface in the direction of the detector (exitance being Lambertian, same radiance flows into every direction before crossing the interface). It is given by:

$$T_{out} = T_{12}(8°)/n^2, \tag{9}$$

where the factor $1/n^2$, independent of the radiance orientation, comes from the change in solid angle due to the refraction of exiting rays through the interface [23].

For a refractive index of 1.5, which is approximately the one of dental composite materials over the visible spectrum of light [21], we have $r_i = 0.596$, $T_{in} = 0.908$, and $T_{out} = 0.426$.

Calibration of the two-flux model

The calibration of the two-flux model is the numerical computation of the absorption and scattering coefficients from the reflectance and transmittance factors measured on a slice of the considered material, for each wavelength, with given thickness *h* assumed to be known. If the optical index is also known or assumed, only *K* and *S* are to be determined.

First, we determine the intrinsic reflectance ρ and transmittance τ of the layer considered without interface, which are related to the reflectance factor *R* and transmittance factor *T* measured according to Eqs. (5) and (6). By considering that $T'_{in} = T_{in}$ and $T'_{out} = T_{out}$, and by denoting $R' = R - r_e$, we obtain:

$$\rho = \frac{R'T_{in}T_{out} + r_i\left(R'^2 - T^2\right)}{\left[r_i\left(R' - T\right) + T_{in}T_{out}\right]\left[r_i\left(R' + T\right) + T_{in}T_{out}\right]} \tag{10}$$

and

$$\tau = \frac{T_{in}T_{out}T}{\left[r_i\left(R' - T\right) + T_{in}T_{out}\right]\left[r_i\left(R' + T\right) + T_{in}T_{out}\right]} \tag{11}$$

By using the notations:

$$u = \sqrt{\left(1 - \rho\right)^2 - \tau^2} \quad \text{and} \quad v = \sqrt{\left(1 + \rho\right)^2 - \tau^2}, \tag{12}$$

according to Eqs. to (4), parameters a and b can be written:

$$a = \frac{1 + \rho^2 - \tau^2}{2\rho} = \frac{u^2}{2\rho} + 1 \quad \text{and} \quad b = \frac{uv}{2\rho} \tag{13}$$

Since, according to Eqs. and (2), we have:

$$\sinh\left(bSh\right) = b\frac{\rho}{\tau}, \tag{14}$$

and thus obtain:

$$S = \frac{2\rho}{huv}\operatorname{arcsinh}\left[\frac{uv}{2\tau}\right] \tag{15}$$

and

$$K = S(a - 1) = \frac{u}{hv}\operatorname{arcsinh}\left[\frac{uv}{2\tau}\right] \tag{16}$$

3. Measurement issues with translucent materials and revision of two-flux model

In Section 2, we introduced the "effective measurement geometry" concept which better depicts the light paths reaching the detector, therefore the interpretations that the parameters of the two-flux model (Kubelka-Munk model and Saunderson correction) should be given. We argue that for a translucent layer through which transmitted light remains mainly directional, the values of the Saunderson correction parameters are far away from the ones given in Section 2 for strongly scattering layers. But before that, we would like to insist on "edge-loss" another important source of error in the measurements [35].

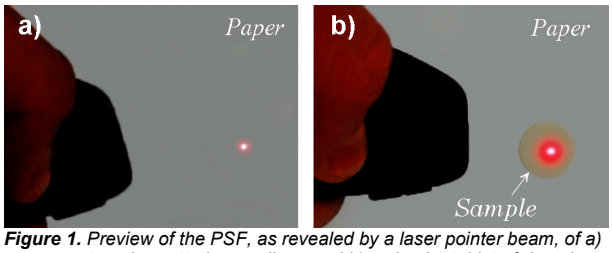

Figure 1. *Preview of the PSF, as revealed by a laser pointer beam, of a) paper, a strongly scattering medium, and b) a circular tablet of dental composite material ('Sample') placed on top of the paper.*

Preventing edge-loss

A frequent measurement issue arises with translucent materials, i.e., materials whose scattering coefficient (in m^{-1}) is low and therefore whose scattering free mean path (in m) is high, due to the fact that any light ray entering the material propagates far away from its entrance point in the medium, a phenomenon which can be assessed by a point spread function (PSF) [17-19]. Figure 1 shows the difference in PSF between a strongly scattering, visually opaque paper, and a weakly scattering, visually translucent dental composite material.

If the instrument illuminates and observes the same area, the light collection system may miss the light emerging out of this area, and the reflectance may be consequently underestimated. In the case of human skin, as skin scatters long visible wavelengths in a weaker way (it is more translucent for red light), the amount of missed light is mainly in this spectral domain and causes what is called the "red-loss" [20]. This does not happen with a strongly scattering medium, as light is mostly backscattered after a short travel into the medium and does not propagate far from the illuminated area. This also does not happen with a transparent material, non-scattering, that light can cross straightforward without deviating laterally from the illuminated area. In order to prevent this underestimation of reflectance or transmittance, the best option is to collect light from an area much larger than the illuminated one. Alternatively, the collection area can also be much smaller than the illuminated one; this second option, implemented in some spectrophotometers (MetaVue or Color i7, from X-rite company, USA), is equivalent to the first one according to the Helmholtz reciprocity principle (or reverse path principle) [26]. The experiments shown in this paper are based on measurements performed with this option. In contrast, some reflectance values reported in Reference [21] are unexpectedly low, and it is possible that they have been measured with similar illumination and collection areas.

Revising the Saunderson Correction

The Saunderson correction as presented in Section 2 assumes that the external irradiance of the sample (illumination), as well as the internal irradiance of the interfaces (light scattered by the material) are Lambertian. With a d:8° measuring geometry, both assumptions are certainly verified when the medium is strongly scattering. They look also verified at first sight in the case of weakly scattering media, but if one pays attention to the light paths across the sample, one would observe that they are much more directional than what is implicitly assumed by the two-flux model: the radiance reaching the detector does not originate from the whole hemisphere of incidence, but rather from a certain cone facing the detection direction, as featured in Figure 2 in the case of the transmission mode. The incident light coming from outside the cone is more likely to be scattered in other directions than the one of the detector, and to be simply ignored from the measurement. Hence, the light captured, especially in transmission mode, rather corresponds to bi-directional, or conical-directional geometry, which considerably modifies the angular distribution of the light concerned at the interfaces.

Let us consider the extreme case where the sample is transparent, i.e., perfectly non-scattering. Only the radiance facing the detector is incorporated into the measurement, and the effective measuring geometry, in both reflectance and transmittance modes, is the 8°:8° geometry (or, almost equivalently, the 0°:0° geometry) [27]. In this case, the parameters used in the Saunderson correction, r_e, r_i, T_{in}, and T_{out}, corresponds to Fresnel reflectance and transmittances at normal incidence, i.e., for a refractive index of 1.5:

$$r_e = r_i = R_{12}(0°) = 0.04 \tag{17}$$

instead of instead of 0.596 in the case of a strongly scattering media, and

$$T_{in} = T_{out} = 1 - R_{12}(0°) = 0.96 \tag{18}$$

instead of $T_{in} = 0.908$ and $T_{out} = 0.426$.

As the sample becomes more scattering, the four-flux model looks preferable [28, 29, 30, 31]. In addition to the two opposite diffuse fluxes considered in the two-flux model, it also considers two opposite directional fluxes, as well as the mutual exchanges between the two types of fluxes. It relies on two absorption and two scattering coefficients, attached to the two kinds of fluxes. The Kubelka-Munk formalism is transposed into a matrix formalism in a rather straightforward way. However, the four-flux model needs four measurements instead of two, which needs affordable but specific equipment.

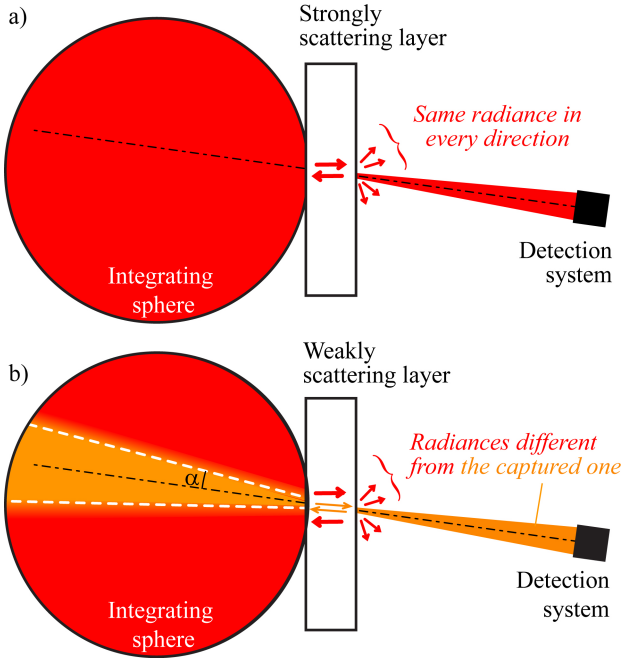

Figure 2. *d:8° measurement geometry used in transmittance mode. a) In the case of a strongly scattering sample, the radiance captured by the detector is formed by flux elements originating from anywhere in the integrating sphere, and it is 1/π times the total Lambertian exitance. b) In the case of a translucent samples, the radiance captured by the detector is formed by flux components originating mainly from a certain cone of half-angle α and follows a rather directional path through the sample; Flux components originating from elsewhere in the sphere mostly contribute to uncaptured radiances.*

For people who prefer to use the two-flux model, in particular because of the limitations of their measurement equipment, we recommend a reevaluation of the terms r_e, r_i, T_{in}, and T_{out} according to the effective measurement geometry, or at least a rough estimation of it (for example by illuminating the sample at normal incidence with a laser pointer beam and observing the cone through which most transmitted light is scattered, this being comparable to the one that contains the incident light able to reach the detector in collimated detection, thanks to the Helmholtz reciprocity principle). The Kubelka-Munk model in itself is not modified, even though the absorption and scattering coefficients stand for "directional" flux components, not for the "diffuse" ones, according to the meaning given to the terms in the four-flux theory [30].

Note that the cone aperture over which light is scattered can be rather large without numerical consequence on the values for r_e, r_i, T_{in}, and T_{out} given in Eqs. (17) and (18). Regarding T_{in} for example, its value for an effective illumination cone of half-angle α (see Figure 2), would be given by

$$T_{in} = \int_0^{\alpha} T_{12}(\theta) L_i(\theta) \sin 2\theta d\theta \Big/ \int_0^{\alpha} L_i(\theta) \sin 2\theta d\theta \qquad (19)$$

where $L_i(\theta)$ denotes the angular radiance within the cone, which is a constant in case of Lambertian illumination and can therefore be ignored.

Since for the refractive index 1.5 considered here $T_{12}(\theta)$ is rather constant when θ ranges from 0° to 45°, we can say that if α is lower than 45°, $T_{12}(\theta)$ is very close to the transmittance of the interface at normal incidence. Same considerations apply to T_{out}.

Likewise, $R_{21}(\theta)$ is rather constant for θ ranging from 0° to 25° and the internal reflectances of the interfaces are close to the Fresnel reflectance at normal incidence [Eq. (17)] for an effective illumination cone of half-angle smaller than 25°.

4. Experimental verification

The dental composite used for this experimental part of this study is the Wave Medium Viscosity B1 shade material commercialized by the Southern Dental Industries company, Australia. Samples of four thicknesses, 0.4 mm, 0.8 mm, 1.0 mm and 1.2 mm, were produced by placing the composite between two glass plates with defined spacing in order to fix the thickness, then hardened by blue L.E.D. light curing unit (1200 mW/cm² during 60 seconds). The sample diameter, determined by the volume of material deposited, is 20 mm. The four samples, placed on top of a drawdown card, are shown in Figure 3. Their translucency is well perceptible through the way the black and white backings appears through. We can also perceive a slight opalescence effect characterized by a bluish aspect on the black backing and a yellowish aspect on the white backing. Their reflectance and transmittance factors were measured with the Color i7 spectrophotometer from X-rite, USA, based on the d:8° geometry in both reflectance and transmittance modes, by choosing the largest illumination area possible (17 mm diameter) and the smallest observation area allowed by the instrument (6 mm diameter). The specular reflection component was included in the reflectance measurements. The refractive index of the material is assumed to be 1.5, the value usually considered for some dental resin composite materials [32].

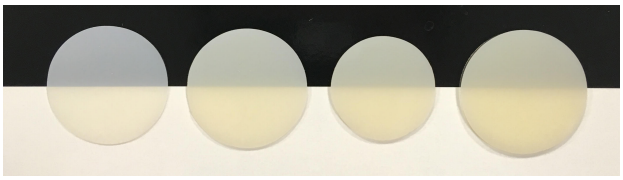

Figure 3. *Samples of Wave Medium Viscosity B1 shade material used for the experiments, with respective thicknesses 0.4 mm, 0.8 mm, 1.0 mm and 1.2 mm, on top of a drawdown card.*

In the calibration step, the absorption and scattering coefficients of the material are computed from the reflectance and transmittance factors of the sample with thickness 0.8 mm, or the one with thickness 1.0 mm, or the one with thickness 1.2 mm (*calibration sample*). The model used for the calibration, then for the prediction of the reflectance and transmittance factors of the samples not used for the calibration (*test samples*), is either the classical two-flux model reminded in Section 2 (the parameters used in the Saunderson correction rely on the assumption of a strongly scattering medium), or the revised model (these parameters are modified to better account for the light orientation at the interfaces, as explained in Section 3). In order to assess perceptually the deviation between predicted and measured spectra, all spectra were converted into CIE 1931 XYZ tristimulus values by considering a D65 illuminant, then into CIE 1976 L*a*b* color coordinates by considering the same illuminant and a perfectly white diffuser as white reference in reflection mode, or void as white reference in transmittance. Spectral deviations are finally assessed by the CIEDE2000 metric, knowing that psychophysical experiments carried out with similar dental materials have determined a visual acceptability threshold in terms of color difference around 2 units (1.8 and 2.25 according to Refs. [33] and [12], respectively), the just noticeable difference being around 1.3 according to Ref. [12].

The CIEDE2000 values between predicted and measured colors, obtained for all combinations {calibration sample / test sample}, in reflectance and transmittance modes, with the classical and revised models, are all shown in Table 1. For all samples, we can observe that the prediction accuracy of the classical two-flux model is rather low: half the CIEDE2000 values (in red) are beyond the acceptability threshold. The revised model (CIEDE2000 values in green) yields a sensible, even sometimes dramatic gain in prediction accuracy, especially in transmittance mode for which the predictions are fairly good. This is also well visible in Figure 4 where the measured and predicted spectral reflectance and transmittance factors of the samples with thickness 0.4, 0.8 and 1.2 mm are plotted, the model being calibrated from measurements on the sample with thickness 1.0 mm. Note that the reflectance and transmittance factors of the sample from which the scattering and absorption coefficients were extracted are perfectly predicted (CIEDE2000 value zero, replaced with a symbol "-" in the table for better reading), because the Kubelka-Munk formulae are reciprocal. This is the reason why the spectra corresponding to the sample with thickness 1 mm have not been plotted in Figure 4. The poorest predictions are obtained in reflectance mode for the thinnest sample (0.4 mm, first line of Table 1), because of a noticeable deviation in short wavelengths (see the reflectance factor in Figure 4.a), probably due to a sensible opalescence effect that a flux model, based on incoherent light theory, cannot predict.

Table 1. CIEDE2000 color distances between predicted and measured reflectance (*R*) and transmittance (*T*) factors[a]

	Calibration sample											
	0.8 mm				1.0 mm				1.2 mm			
Test sample	*R*		*T*		*R*		*T*		*R*		*T*	
0.4 mm	8.9	2.2	4.6	0.6	9.9	2.8	5.5	0.8	10.4	3.3	6.0	0.8
0.8 mm	-	-	-	-	2.2	0.8	1.8	0.4	3.2	1.6	2.7	0.4
1.0 mm	2.8	0.8	2.2	0.4	-	-	-	-	1.3	0.9	1.2	0.1
1.2 mm	5.0	1.7	4.1	0.5	1.5	1.0	1.4	0.1	-	-	-	-

[a] predictions made for the sample specified on the left of the row with the classical model (red numbers) and the revised model (green numbers), calibrated with the absorption and scattering coefficients computed from the calibration sample specified on top of the column.

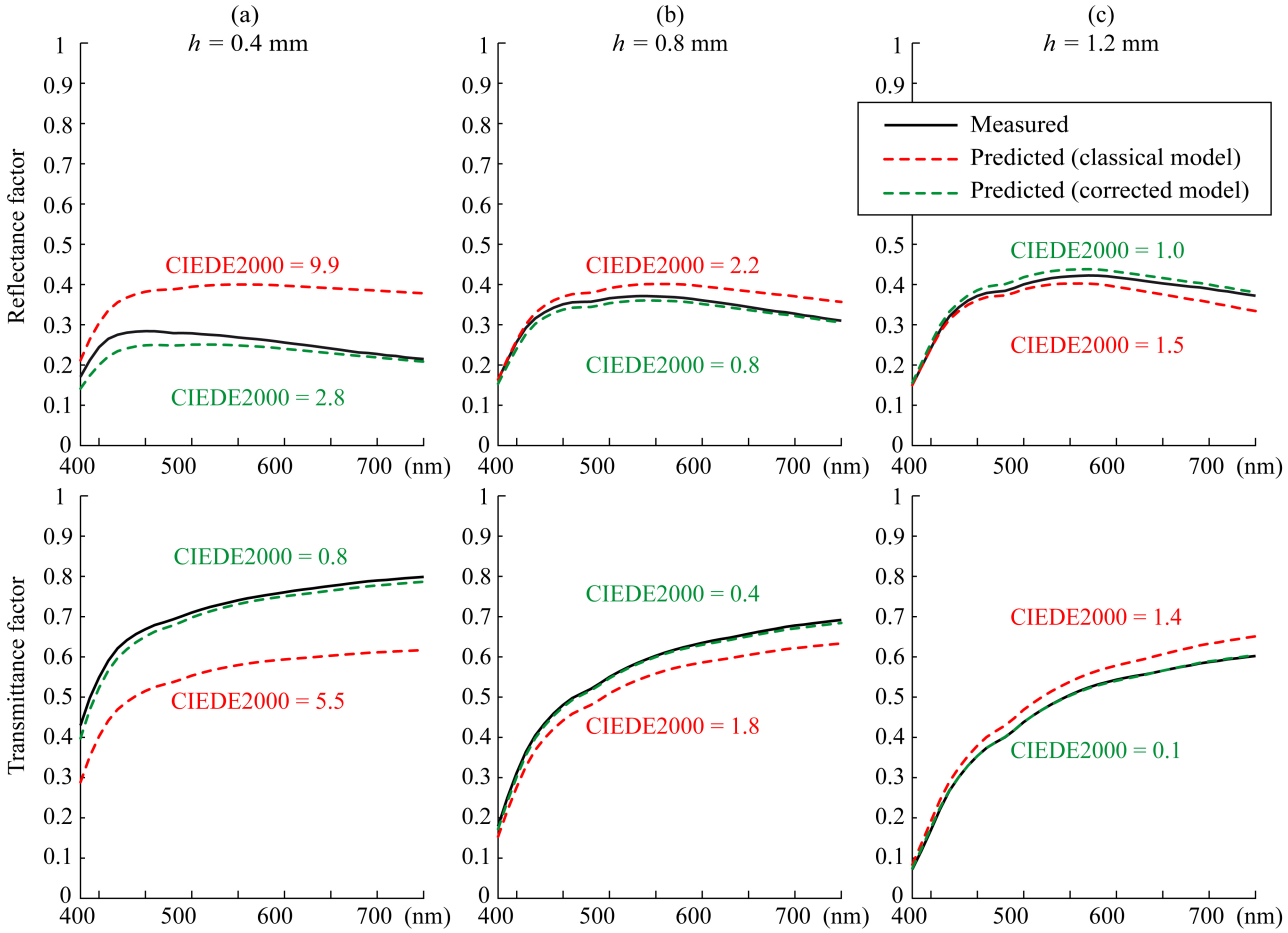

Figure 4. *Reflectance and transmittance factors measured (black solid lines) and predicted by the classical two-flux model (red dashed lines) or the revised model (green dashed lines) for dental composite material samples with thickness (a) 0.4 mm, (b) 0.8 mm, (c) 1.2 mm, while the absorption and scattering have been computed from reflectance and transmittance factor of the sample with thickness 1.0 mm. The CIEDE2000 values are the equivalent color distance between the predicted and transmitted spectra, for each model (indicated by the color).*

Since we have four samples from which the model can be calibrated, we can ask which one provides the best predictions. It seems that calibration from the sample with thickness 0.8 or 1.0 mm yields the best predictions for the thinnest and thickest samples. It is not surprising that predictions become poorer as the difference between the thickness of the calibration sample and the one of the test sample increases. Despite the gain in accuracy achieved by revising the model's parameters, the two-flux model still remains limited in its capacity to model the light propagation through samples over a large range of thicknesses. It is certain that, beyond a certain thickness, the layer will become strongly scattering (every flux initially collimated is finally strongly scattered after a long travel distance in comparison to the scattering free mean path length, and becomes a lambertian flux). It thus gets a more opaque appearance, and the classical two-flux model should apply. Notice, however, that the absorption and scattering coefficients computed from measurements on a "very thick" layer would be characteristic of the propagation of diffuse light and would therefore yield poor predictions for a thin layer on which measurements contain almost no diffused flux component.

Nevertheless, we could verify that the revised model calibrated from the sample with thickness 1 mm performs rather well up to a sample thickness of 3.4 mm. These higher sample thicknesses could be achieved by stacking the four samples used so far, in optical contact done with water. We verified that water, despite its rather low refractive index (1.33) compared to the one of the material (1.5), provides good enough optical contact, by stacking together the samples with thickness 0.4 mm and 0.8 mm and comparing the measured reflectance and transmittance factors with the ones of the sample with thickness 1.2 mm. The deviation between the two

was very small: an equivalent color difference CIEDE2000 of 0.32 unit has been observed in reflectance mode, and 0.40 unit in transmittance mode. Hence, we obtained the samples listed in Table 2. The low CIEDE2000 units assessing the deviation between predicted and measured spectra indicate that the model is fairly accurate in transmittance mode. In reflectance mode, the prediction accuracy is poorer, but not aberrant.

Table 2. CIEDE2000 color distances between predicted and measured reflectance and transmittance factors[a]

Sample thickness in mm (composite combination)	Reflectance	Transmittance
0.4	2.8	0.8
0.8	0.8	0.4
1.0	0	0
1.2	0.6	0.3
1.2 (0.4 + 0.8)	0.9	0.1
1.4 (0.4 + 1.0)	1.2	0.3
1.6 (0.4 + 1.2)	1.8	0.3
2.2 (0.4 + 0.8 + 1.0)	2.8	0.7
2.4 (0.4 + 0.8 + 1.2)	3.2	0.8
2.6 (0.4 + 1.0 + 1.2)	3.4	0.6
3.4 (0.4 + 0.8 + 1.0 + 1.2)	4.2	0.5
Average	2.0	0.4

[a] predictions made with the revised model, calibrated with the absorption and scattering coefficients computed from the 1 mm thick sample for various samples and stacks of samples in optical contact.

5. Conclusions

This work confirms that the Kubelka-Munk model with Saunderson correction is capable of rather accurate predictions of the reflectance of thin slices of dental composite materials, as it has been already observed by using a different calibration method based on samples in optical contact with black and white backings [11-16]. It also shows that good prediction accuracy can be achieved for the transmittance, provided the light transfers at the interfaces of the medium are carefully evaluated using an "effective measurement geometry", this latter being sensibly different from the "instrument geometry" in case of weakly scattering layers. We showed that for the pieces of weakly scattering dental materials considered in this paper, the light captured by a spectrophotometer based on a d:8° geometry mainly follows a rather directional path through the material, not far from the normal of the sample. It is therefore more correct to use Fresnel reflectances and transmittances for normal incidence as parameters in the Saunderson correction rather than the hemispherical ones classically used for strongly scattering media. We also showed through experiments that performing this reevaluation of the Saunderson correction parameter considerably improves the prediction accuracy of the model, both in reflection and transmission modes. One must be aware that the scattering and absorption coefficients computed in this way are characteristic of the propagation of this rather directional light and not on the more diffused light that would propagate in a much thicker slice of material. For achieving good predictive performance over a broad range of thicknesses, a more rigorous model based on the radiative transfer theory [34], or on the four-flux model if one wants to maintain a formalism closer from the one of the two-flux theory [29,30], would be much preferable.

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