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Diaphaneity diagrams for analyzing the validity range of analytic optical models

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Abstract

Recent attempts to determine the optical properties (absorption and scattering coefficients) of translucent materials from affordable instrumentation converged on fixed-geometry spectral measurements and two-flux or four-flux photometric models. They are appealing at an industrial scale due to the measurement simplicity and computational efficiency. However, it is difficult to assess the accuracy of the method because of a lack of ground truth values for the expected coefficients with a given material. In this paper, we address the problem using synthetic data: given optical coefficient values, we predict the measurable reflectance and transmittance of slices of materials using two models — a Monte Carlo (MC) model, which serves as a reference, and the two-flux Kubelka-Munk model. A large number of coefficient values are tested, allowing to identify the ranges of values for which the two-flux model predicts measurable quantities consistent with those predicted by MC, and thus to determine its range of validity. To better observe the general trends, we introduce a graphical representation system, called a "diaphaneity diagram," where each sample is represented by a point based on its measurable reflectance and transmittance. By varying the optical coefficients, the two models draw lines whose proximity allows us to visualize their agreement. Then, for some material sample whose reflectance and transmittance have been measured, it is easy to see if its diaphaneity point is located in a region of the diagram where the two-flux model agrees with the MC model, and thus whether two-flux model can provide relevant optical coefficient values.

Categories and Subject Descriptors (according to ACM CCS): I.3.5 [Computer Graphics]: Computational Geometry and Object Modeling—Physically based modeling; I.6.4 [Computer Graphics]: Model Validation and Analysis—

1. Introduction

Several application domains need reliable and practical methods to control the appearance of objects made of translucent materials, such as additive manufacturing resins, textiles, polymers, dental materials, and biologic tissues. Although it is still often made with an empirical way, scientific methods based on optical models are being developed in order to predict appearance attributes such as color as a function of the material's shape and properties.

Various methods exist to determine these properties from the measurement of a limited number of samples with known geometry [FJM*20]. Among these methods, the Saunderson-corrected Kubelka-Munk two-flux model [KM31, Sau42, Kub48] is popular due to its compatibility with commercial instrumentation and simple closed-form analytical formalism. This two-flux optical model relies on the assumption that the light fluxes entering the slab, scattered in the material, and exiting the slab are orthotropic, i.e., Lambertian, an assumption that is never met since it requires bi-hemispherical reflectance and transmittance measurements, which do not exist for reflectance. Instead, a directional-hemispherical (or equivalently hemispherical-directional) geometry is often used. Two measurements are made: either the reflectance and transmittance factors of the slab, or the reflectance factors of the slab in optical contact with black and white backgrounds. This directionality of the incident (or observed) flux reduces the compatibility between the measurement and the model, except for material of high optical thicknesses for which light is strongly scattered just after entering the material. Hence, for translucent materials, the model accuracy depends on the intrinsic properties of the measured sample [Duv23].

The objective of this work is to get a better understanding of the circumstances in which this analytic model gives accurate values for the desired optical properties. For this purpose, ground truth values are needed. In absence of a large set of samples whose optical parameters would be certainly known, covering a large range of absorptance and translucency, we follow a different approach based on synthetic data: we perform numerical simulations of slabs with selected optical properties for which the reflectance and transmittance measurements are simulated with a geometry available in commercial instruments. These simulations are based on the radiative transfer equation through a Monte Carlo method [TJS*24]. They are computationally demanding but are based on a robust, complete and well-established theory, and can be considered as a ground truth. The radiometric quantities obtained from the Monte Carlo simulations and from the two-flux optical model can then be compared.

To facilitate this comparison, we introduce a graphical representation that we call a *diaphaneity diagram*. We let *diaphaneity* refer to the intrinsic translucency of a material, independently from its shape or thickness. This graphical representation has been inspired from the one presented by Iser et al. [IRN*22]. We adapted this concept to account for different types of spectrophotometric measurements. We detail this graphical tool in Sec. 2, and present the comparison between the two-flux model and the Monte Carlo method to map intrinsic optical parameters in Sec. 3.

2. Diaphaneity diagrams for translucent materials

The graphical representation for translucent materials we use in this work is schematized in Fig. 1. At a given wavelength, every slice of material is represented by one point (x,y) in the diagram, which features the optical properties of the material at that wavelength. Different quantities can be used for coordinates x and y, leading to different types of diaphaneity diagrams: in the work of Iser et al. [IRN*22], x and y are custom measurements of light intensity of slabs placed in front of black and white backgrounds. In this work, we rather use quantities that are compatible with commercial instrumentation and predictable through analytic optical models. A first one, called RT-diaphaneity diagram, relies on the reflectance and transmittance factors, R and T in hemispherical-directional measurements geometry, with observation at 8° – noted *d:8°* geometry – of smooth samples. The position in the diagram is defined by $(x,y) = (R,T)$. The second type, called R_kR_w-diaphaneity diagram, relies on the reflectance factors, R_k and R_w, with the same measurement geometry, of smooth samples in optical contact with black and white backgrounds respectively. The position in the diaphaneity diagram is $(x,y) = (R_k, R_w - R_k)$

In both diagrams, the vertical axis corresponds to various levels of translucency: from completely opaque to clear materials. The horizontal axis corresponds to various levels of scattering: from non-scattering to strongly scattering materials. Transparent materials are located along the vertical axis, and milky materials (non-absorbing but possibly scattering materials) are on the diagonal.

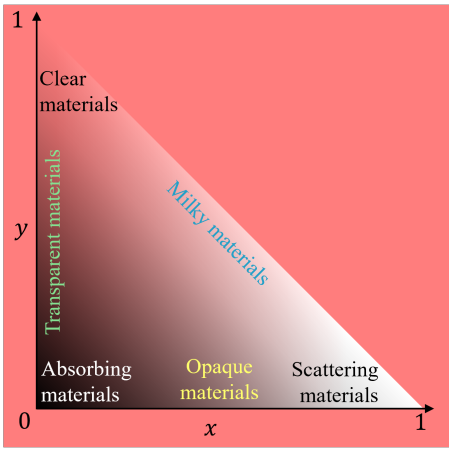


Figure 1: Diaphaneity diagram.

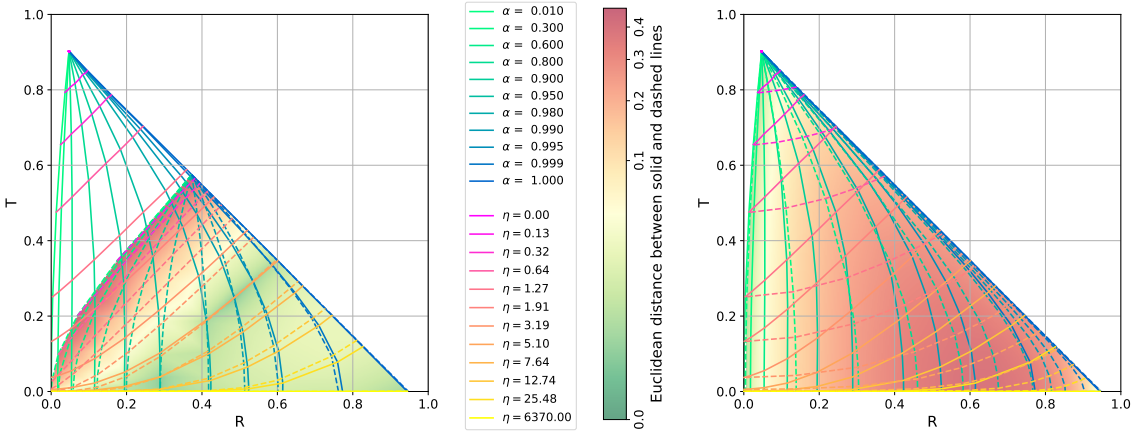
The objective of these diaphaneity diagrams is to derive both qualitative assessments on the appearance of a material and quantitative estimation of its intrinsic optical properties from its position in the diagram. In the next section, by considering various optical properties, we predict radiometric quantities with the MC model (ground truth values), and the two-flux model, and display the corresponding points in diaphaneity diagrams in order to see when the two-flux model deviates from the MC model.

3. Gridding the diagrams with iso-parameter lines

In this section, we consider a wide range of virtual materials of various intrinsic optical properties. For each set of properties, measurable radiometric quantities are predicted with the Monte Carlo model (ground truth values) and the two-flux model. The predicted quantities yield two points in the diaphaneity diagram, one for each model, whose proximity is measured. We follow this approach in turn with the RT-diaphaneity diagram is detailed in Sec. 3.1, and the R_kR_w-diaphaneity diagram in Sec. 3.2.

3.1. RT-diaphaneity diagram

We consider a smooth slice of material of set optical properties: albedo α and optical depth η. Its reflectance and transmittance factors are estimated from Monte Carlo random walk simulations based on the radiative transfer equation. The considered geometry is d:8°, the specular component is excluded. The Monte Carlo simulations rely on the Henyey-Greenstein phase function, and on the Fresnel equations for the air-sample interface. We simulate isotropic scattering, as in the two-flux model, by setting the asymmetry parameter



(a) (b)

Figure 2: RT-diaphaneity diagrams estimated for materials of refractive index $n = 1.595$, albedo α, and optical depth η. The iso-parameter lines are predicted by the MC model (solid lines), and the two-flux model (dashed lines), and the color background indicates the deviation between them. The Saunderson correction in the two-flux model accounts for two different light-flux geometries at the interface: (a) d:8°; (b) bi-directional geometry with an illumination and observation at 8°.

to $g = 0$. For each (α, η) properties we obtain one dot in the diagram. By varying one of the parameters, we obtain iso-parameter lines in the diagram. Multiple iso-α and iso-η are displayed in solid lines in Fig. 2a gridding the RT-diaphaneity diagram.

The two-flux model was implemented as described by [Héb22] (in Sec. 6.1.2.) It depends on the Kubelka-Munk coefficient of absorption K, and scattering coefficient S. They can be converted from α and η using a transformation from Thennadil [The08]: considering a slice of thickness h, its extinction coefficient is $\mu_t = \eta/h$, its scattering and absorption coefficients are $\mu_s = \alpha\mu_t$ and $\mu_a = \mu_t - \mu_s$ respectively, and the transformation gives

$$K = 2\mu_a, \qquad S = 3\mu_s(1-\gamma)/4, \tag{1}$$

where the γ parameter was optimized to get similar values between Monte Carlo and the two-flux model when the slice is opaque: when the Monte Carlo simulations and the two-flux model should behave similarly, since the K and S coefficients assume diffuse fluxes. The value was found to be $\gamma = 0.209$ for a material of optical index $n = 1.595$. In the end, this method is independent from the thickness h since the two flux model takes as input Kh and Sh. The two-flux model relies on the Saunderson correction ([Héb22], Sec. 6.3.2) to account for the light transfers at the interfaces with air, described by the coefficients r_s, r_i, T_{in} and T_{out}. With $n = 1.595$ and for a d:8° measurement geometry, specular component excluded, these are: $r_s = 0$, $r_i = 0.6484$, $T_{in} = 0.8945$ and $T_{out} = 0.3724$.

The iso-parameter lines obtained with the two-flux model are displayed in dashed lines in Fig. 2a. The euclidean distance between the two-flux estimated iso-parameter lines and the Monte Carlo ones is displayed as a colored map. When the optical depth is high (yellow curves), the iso-parameter lines from the two-flux model are rather close to the Monte Carlo ones since the light is mostly diffuse, the two-flux model is then rather accurate in this area of the diagram. Note that the two-flux model does not cover the same range of reflectance and transmittance factors as the Monte Carlo simulations. This is because the model assumes orthotropic light fluxes, whereas, for the clearest materials, the light fluxes at the interfaces are mostly directional. In this case, the Saunderson correction in the two-flux model can be modified to account for directional light fluxes at the interfaces, by replacing in the equations r_s, r_i, T_{in}, and T_{out} by the coefficients estimated for a directional illumination and observation at 8°, specular component excluded: $r_s = 0$, $r_i = 0.0526$ and $T_{in} = T_{out} = 0.9474$.

The diaphaneity diagram obtained with this directional assumption, is displayed in Fig. 2b. In this diagram, the conversion of (μ_a, μ_s) into (K, S) is performed with $K = \mu_a$ and $S = \mu_s$. The advantage of this model is that it covers the whole reflectance and transmittance factor range possible, and the optical property estimation is accurate when the material is transparent. Yet, other conversions of (μ_a, μ_s) into (K, S) need to be investigated to improve the accuracy of this two-flux model.

3.2. $R_k R_w$-diaphaneity diagram

The reflectance factors, R_k and R_w in d:8° geometry (specular component excluded), of a smooth slice in optical contact with black and white backgrounds, are simulated for various

α and η parameters with a similar Monte Carlo method as described in Sec. 3.1, considering a perfect diffuser for the background. The iso-parameter lines issued from these simulations are displayed in solid lines in Fig. 2b. These lines are compared with the ones issued from the two-flux model for slabs in optical contact with a background, displayed in dashed lines in Fig. 3. This model was implemented as described by [Héb22] (in Sec. 6.2). The conversion of (α,η) into (K,S) is performed with Eq. 1 with the same coefficient $\gamma = 0.209$. The Saunderson correction in the two flux model relied on the same coefficients r_s, r_i, T_{in}, and T_{out} as in Sec. 3.1 for a d:8° geometry.

In the diagram of Fig. 3, the opaque layers are located near the horizontal axis, where the difference between the reflectances on the white and black backgrounds vanishes. This means that the material either absorbs or scatters a lot, which corresponds to high optical depth (yellow curves on the graph). On this axis, if R_k is high, the material is highly scattering, which corresponds to a high albedo (blue curves). Near the vertical axis, the reflectance on the black background is low: the material is transparent (non-scattering), the albedo is therefore low (green curves). Overall, the R_kR_w-based to flux model has a better accuracy than the RT-based one since the diffuser in optical contact with the slab increases the compatibility between the two-flux model assumptions and the effective measurement geometry.

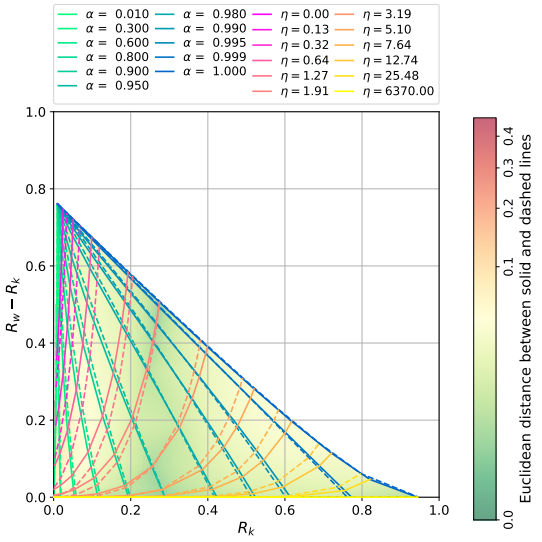


Figure 3: R_kR_w-diaphaneity diagrams estimated for materials of refractive index $n = 1.595$, in optical contact with black and white backgrounds of intrinsic reflectance $\rho_k = 0.03$ and $\rho_w = 0.93$ respectively. The iso-parameter lines are predicted by the MC model (solid lines), and the two-flux model (dashed lines), and the color background indicates the deviation between them.

4. Conclusion and discussion

The diaphaneity diagrams are viewed as a tool to easily visualize the optical properties of a material from simple spectrophotometric measurements. Thanks to our gridding with iso-coefficient lines, they can also be used to check whether the two-flux model is accurate for any slice of material. It suffices to measure either R and T, or R_k and R_w on the slice, to place the point in the corresponding diaphaneity diagram, and to see if the point is located in a region where the two-flux model agrees with the MC model considered as ground truth. The displayed diaphaneity diagrams are valid for one refractive index and one instrument geometry. They can be extended to other refractive indices and standard geometries and allow to evaluate the accuracy of more complex models such as four-flux models.

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