Stratum Corneum Light Confinement: Monte Carlo Verification

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Abstract: *Significance*: The epidermis, the outermost layer of the skin, plays a crucial role in protecting the body from UV radiation, chemical substances, and physical trauma. Its top layer, the stratum corneum (SC), consists of dead skin cells with low water content (~20%), creating a refractive index gradient between the SC and underlying tissue. This gradient traps light within the SC layer, but its impact on light propagation in tissues remains largely unexplored. *Aim*: The study investigates how refractive index variations in the skin influence light propagation in tissues. *Approach*: Monte Carlo (MC) light transport simulations were performed in media with and without refractive index mismatches. *Results*: Light confinement in the SC increases the fluence rate by 12-35% compared to underlying tissue, particularly when the underlying tissue has low diffuse reflectance. This effect is most pronounced when the SC thickness exceeds the reduced scattering length (~150-600 μm for visible light). Such thicknesses occur in glabrous skin (palms, soles) and thickened areas like calluses and corns. *Conclusions*: By comparing MC simulations, we attribute this light confinement to the SC's high refractive index due to its low water content. This stratum corneum light confinement (SCLC) phenomenon may lead to an inaccurate estimation of light distribution, resulting in errors in some skin diagnostic parameters measured via diffuse reflection, such as water and total hemoglobin content, and blood oxygenation.

1 INTRODUCTION

The epidermis is the outermost layer of the skin, and it plays a crucial role in protecting the body from external insults such as UV radiation, chemical substances, and physical trauma. The epidermis can be subdivided into two sublayers: non-living and living epidermis. The non-living epidermis (~20 μm thick) consists of only dead squamous cells, which are highly keratinized with a high lipid (~20%) and protein (60%) content and a relatively low (~20%) water content (Bashkatov, 2011). In terms of water content, the stratum corneum radically differs from the underlying skin layers, which have much higher water content—the typical water content in these live skin layers is 70%.

Due to the significant difference in refractive index between proteins/lipids and water, skin tissues can be stratified into two layers: stratum corneum with the higher refractive index (n = 1.467) and all other underlying tissue with lower refractive index (n = 1.383).

The low water content of stratum corneum has significant implications on water content imaging (Saiko, 2023a), particularly for thickened areas (corns and calluses). While the light propagation in multilayer skin models has been studied analytically (Sergeeva, 2024; Phillips, 2009; Liemert, 2017), numerically (Chang, 2023; Sadeghi, 2022; Yudovsky, 2011; Grossweiner, 1992, Dehghani, 2003), and experimentally (Farrell, 2001), the effect of refractive index gradient on skin optics has not been adequately explored so far, which may have certain implications for actively developing optical medical devices and consumer health fields. In a recent development, Saiko (Saiko, 2023b) developed an analytical approach to account for the refractive index gradient and predicted the light confinement in the stratum corneum.

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The current work aims to elucidate the impact of a significant gradient of water content and, consequently, the gradient of the refractive index of the skin layers in tissues, which can help more accurately describe the light propagation in tissues. In this study, we validate the model predictions (Saiko, 2023b) with established Monte Carlo simulations of light propagation (specifically the *gpumcml* program (Alerstamet, 2010)).

2 METHODS

2.1 Tissue Model

We have performed Monte Carlo simulations of light transport in a two-layer model (the stratum corneum and underlying tissue) to elucidate the peculiarities of light propagation in the proposed model.

2.1.1 Index of Refraction

The refractive indexes of tissue structure elements, such as the fibrils, the interstitial medium, nuclei, cytoplasm, organelles, and the tissue itself, can be derived using the law of Gladstone and Dale, which states that the resulting value represents an average of the refractive indices of the components related to their volume fractions. Water content varies in different skin layers. To account for the impact of water content on the refraction index, a simple approach was proposed by (Troy, 2001), which assumes that the tissue consists of protein and water. If proteins have a refractive index of 1.5, we get the following expression, which is a generalized version of (Troy, 2001), which used water content, c_w=0.7,

$$n_{skin} = (1 - c_w)1.5 + c_w n_{water} \quad (1)$$

Water's refractive index in the spectrum's visible range (380 - 700 nm) can be estimated as 1.333 (Hale, 1973). However, its wavelength-dependent approximations can be used to account for the dependence on the light wavelength if necessary. Due to the significant difference in refractive index between proteins and water, tissues can be stratified into two layers: stratum corneum with a higher refractive index and all other underlying tissue with a lower refractive index. They will be denoted by subindexes 1 and 2, respectively. Subindex 0 will correspond to the surrounding medium (air). Note that while stratum corneum has a high lipid content, it does not change our assumptions, as lipids also have a high refractive index. We have calculated the refractive index for tissue layers using Eq.1. We considered two scenarios: c_w=0.7 (n=1.383) and c_w =0.2 (n=1.467).

2.1.2 Underlying Tissue Optical Parameters

As we are interested primarily in the effect of refractive index gradient, we have selected three sets of underlying tissue parameters to emulate the low, medium, and high reflectance R (approximately 0.1, 0.3, and 0.5, respectively). The (μ_a, μ_s) values were set to (17cm^{-1}, 80cm^{-1}), (9cm^{-1}, 180cm^{-1}), and (5cm^{1}, 275cm^{-1}), respectively. The anisotropy factor, g, was set to 0.7.

2.1.3 Stratum Corneum Layer Thickness

We selected seven stratum corneum (SC) layer thickness values to emulate a broad range of physiological conditions: d= 20, 50, 100, 200, 500, 1000, and 2000μm.

2.1.4 Stratum Corneum Optical Parameters

We have selected one scenario for the absorption coefficient in stratum corneum: μ_a= 5cm^{1}, which corresponds approximately to flesh absorption at 400nm. We selected three values for the reduced coefficient of scattering: 60, 30, and 15 cm^{-1}. To emulate the effect of different wavelengths (their relative size compared with the scatterer size), we have considered three values for scattering anisotropy: g = 0, 0.4, and 0.8. Thus, we generated three values of (μ_s, g) for each respective μ'_s. As we expect that the observed phenomena will depend on the SC layer thickness in comparison with the scattering transport length and reduced scattering transport length, we selected parameters d, μs, and g to cover all possible relationships between SC layer thickness and the scattering transport length and reduced scattering transport length.

2.2 Monte Carlo Simulations

Using the GPU MCML Monte Carlo software (Alerstamet, 2010), we simulated light propagation in a two-layer model to validate the results of the analytical prediction. The primary model is the semi-infinite tissue (d_2=6mm, n_2=1.383) covered with the stratum corneum layer (n_1=1.467) with thicknesses described in the 2.1.3 section. In total, 3x3x3x7=189 scenarios were simulated.

To elucidate the impact of the refractive index gradient, we have also simulated a scenario without a water content gradient (matched SC/underlying tissue

boundary). Namely, we set n_1=n_2=1.383 (matched SC/underlying tissue boundary) for the same value of the SC absorption coefficient (μ_a= 5cm-1). In total, 3x3x3x7=189 scenarios were simulated and were used as a baseline.

Overall, we simulated 2x3x3x3x7=378 scenarios. From the Monte Carlo simulations, we obtained diffuse reflectance R_d and the dependence of flux intensity on the depth $\Phi(z)$. We used 10^8 photons for each simulation. Resolutions in vertical and lateral directions were set to 10μm and 100μm, respectively.

3 RESULTS

We have calculated the fluence rate around the SC/underlying tissue interface (20μm above and 1mm in the underlying tissue). Examples of the light distributions are depicted in Fig. 1.

To characterize the fluence rate behavior at the interface and below the interface in the underlying tissue, we have calculated the jump in the light intensity over the SC/underlying tissue interface and the slope of the fluence rate in the underlying tissue just below the interface (termed as "gap"). The gap was defined as,

$$gap = (I_+ - I_-)/I_- \quad (2)$$

Here, I_+ and I_- are light flux just above (I_+) and just below (I-) the SC/underlying tissue interface.

In Fig. 2, one can see the dependence of the gap on the SC thickness for all (μs', g) scenarios for matched (dashed lines) and mismatched (solid lines) boundaries for μ_a=5cm^{-1}. Panels are arranged with increasing g (horizontally) and μ_s' (vertically).

As predicted by the analytical model, mismatched boundaries demonstrate a very significant effect on the gap. From Fig. 2, one can see that the gap is approximately 5x larger in the case of the mismatched boundary where n_1 = 1.467 for the stratum corneum and n_2 = 1.383 for the underlying tissue (see, for example, panel 3c, where for R=0.1, the gap is on the scale 0.02 vs. 0.15 for 20μm thickness).

One can see that the gap dependences on R and g are quite significant. As expected, lower reflectance of the underlying tissue, R, translates into more significant gaps. Also, for realistic anisotropy factors (g is around 0.7 in biological tissues), the gap increases with an increase in g. Conversely, the gap decreases as μ_s' increases.

4 DISCUSSIONS

Our analysis shows we can expect several noticeable effects caused by the mismatched boundary between the stratum corneum and underlying tissues.

In particular, it is known that the light intensity is amplified under the surface, which can be described by the ratio of under-the-surface light intensity to the external light intensity. In the case of a matched boundary, the ratio will be close to $1+R$ (forward and backward fluxes). However, the ratio typically has higher values (amplification) than predicted by $1+R$ for mismatched boundaries. In the proposed two-layer model, we have an additional amplification. The light intensity in the SC layer is noticeably higher than just below the interface with underlying tissues, as demonstrated by Fig. 1 and 2. This phenomenon can be attributed to several factors. The first factor is the higher value of the refractive index of the stratum corneum. It increases the overall light intensity under the air/SC interface. However, the light intensity in the stratum corneum layer is noticeably (10-30%) higher than in the underlying tissue layer (see Fig. 2). We have conducted the baseline MC calculations to investigate this phenomenon for the matched boundary between SC and underlying tissues. In this case, the change (gap) is significantly smaller (see Fig. 2). Thus, we can attribute the effect primarily to the mismatched boundary between SC and the underlying tissue and refer to it as the confinement of light in the stratum corneum layer.

The light confinement in the SC layer is similar to fiber optics. Total internal reflections of the light on the interfaces with air and underlying tissues cause it. In particular, the critical angles on these interfaces are $\varphi_{c,a}=arcsin(1/n_{10})$ and $\varphi_{c,ut}=arcsin(1/n_{12})$, respectively. The core differences with fiber optics are that a) instead of highly transparent media (fiber optics), we have a highly scattering media, b) instead of a 1D case (light propagation along an axis in the optical fiber), we have a 2D case (light propagation in the x-y plane), and c) critical angles on both surfaces are not identical. However, a broad range of similar phenomena should likely be observed. For example, it should result in a broadening of the point spread function (PSF), which is caused by the fact that the SC acts as a light guide in the x-y plane. Also, similarly to light leakage due to fiber bending, the same phenomena can be expected to be observed on curved surfaces like heel skin.

As one can see from Fig. 2, the confinement effect is more noticeable for low values of the diffuse reflectance R. It does make sense, as in this case, the underlying tissue is a less significant source of

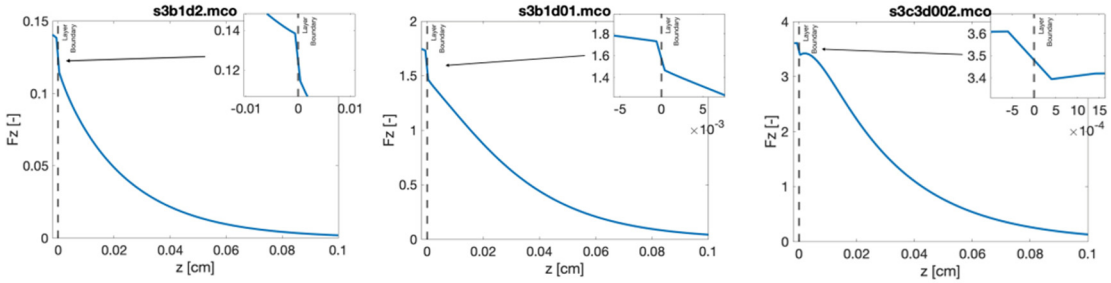

Figure 1: Examples of the fluence rate depth dependence at the SC/underlying tissue interface. (a) with a stratum corneum thickness of 2000 µm, (b) 100 µm, and (c) 20 µm.

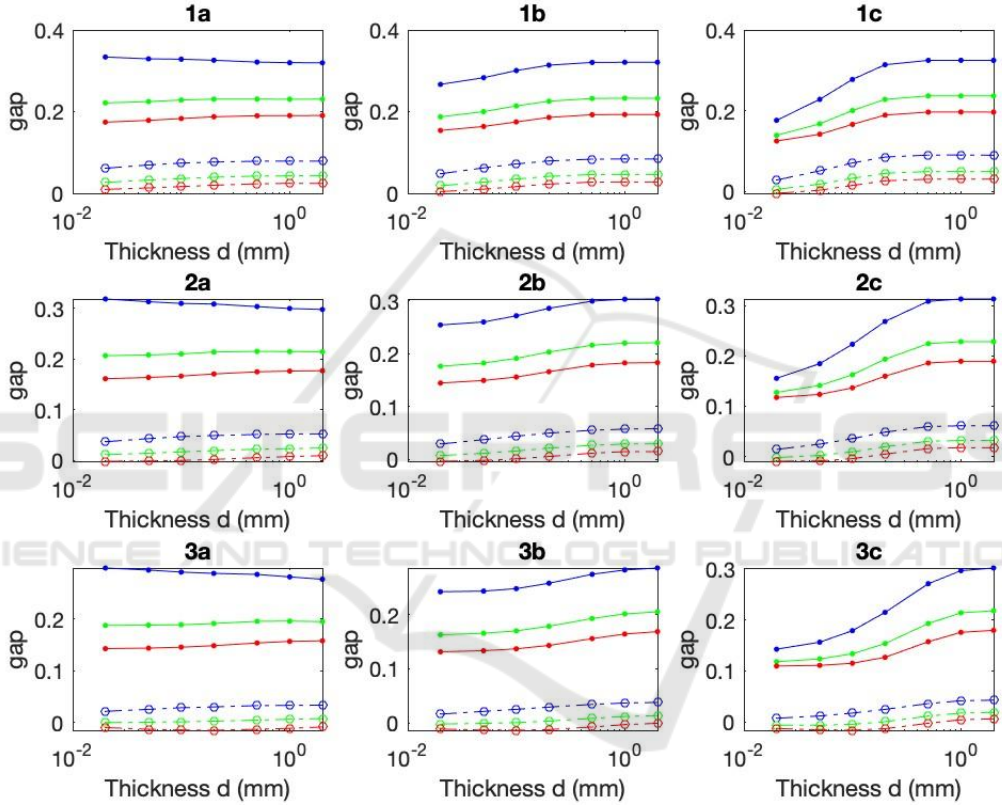

Figure 2: Dependence of the gap on SC thickness d in all (μ_s', g) scenarios for no mismatch (dashed lines) vs. mismatch (solid lines) boundary conditions for various underlying tissue reflectance R. R = 0.1 (blue lines), 0.3 (green lines). 0.5 (red lines). Panels are arranged with increasing g (horizontally) and μ_s' (vertically).

recycled photons for the stratum corneum layer. Thus, most recycled photons come from the total internal reflection on the interfaces between stratum corneum/air and stratum corneum/underlying tissues. For high diffuse reflectance, the underlying tissue is the primary source of recycled photons compared with relatively weak total internal reflectance on the stratum corneum/underlying tissues interface. Thus, the confinement effects (e.g., the additional amplification) are masked by stronger mechanisms (photon injection from the underlying tissues).

Also, the effect depends significantly on the thickness of the stratum corneum layer. In particular, for small (compared with the distance between consecutive scatterings) thicknesses, the photons that enter the stratum corneum from the air pass through the SC layer without experiencing total internal reflection. The same applies to the significant part of photons entering the SC layer from the underlying tissues. As there is no total internal reflection for photons entering from the underlying tissue, all photons from the underlying tissue (other than a

minute fraction of specularly reflected ones) will enter the SC layer; however, just photons with an angle of incidence $\varphi > arcsin(1/n_2)$ will experience total internal reflection on the SC/air interface (the critical angle is 46.3° for n_2=1.383). All others escape the SC through the SC/air interface immediately. However, even a small fraction of photons that experienced total internal reflection on the air/SC interface will immediately exit the SC layer on the SC/underlying tissue interface. Thus, the light confinement will be minimal. In this case, photons within the tissue almost do not feel the presence of the SC layer.

As the SC layer thickness increases, the entering photons start experiencing scattering events. In this case, the light becomes homogenized across various directions in the SC layer. If the thickness is larger than the reduced scattering length, the photon that enters the SC layer from any direction will be homogenized in the SC layer. Thus, the share of oblique photons, which experience total internal reflection in the SC layer, will increase. As a result, the confinement will increase to its maximum value, as confirmed by Monte Carlo simulations (Fig. 2).

As the reduced scattering coefficient for the SC is on the scale 15-70 cm^{-1} in the visible range of the spectrum1, the light confinement phenomenon is maximal in stratum corneum layers with a thickness of at least 150μm and 600μm in blue and red ranges of the spectrum, respectively. These values are typical for the glabrous skin of palms and soles and thickened epidermis like calluses and corns. These estimations were confirmed by Monte Carlo simulations (Fig. 2). However, the effect is almost absent for isotropic (Rayleigh) scattering, which can be strong for shorter wavelengths (<500nm).

The predicted phenomena (the stratum corneum light confinement or SCLC) may have implications for applications in biospectroscopy and bioimaging. There are several possible mechanisms. Firstly, it may impact the sampling/interrogating depth. For example, one can see that for the small diffuse reflectance, the contribution of the SC may dominate in the total reflectance, which may skew certain measurements. Secondly, it may impact the point spread function, which, in turn, may impact the dependence of the reflected light as a function of source-detector distance in spatially resolved spectroscopy. For example, current consumer-grade tissue oxygenation sensors (like Oura ring) can often be interchangeably deployed on non-glabrous and glabrous skin, characterized by a much thicker stratum corneum layer. These phenomena will be explored in future work, where we plan to use Monte Carlo simulations of light propagation in tissues to identify other possible effects of light confinement in stratum corneum on measurements of water and total hemoglobin content and blood oxygenation.

5 CONCLUSIONS

Monte Carlo simulations confirmed light confinement in the stratum corneum layer. The light in the stratum corneum is confined between two interfaces: air and underlying tissues. The effect can be attributed to the high refractive index of the stratum corneum caused by low water content, compared with underlying tissues and scattering in the stratum corneum layer. Light confinement in the stratum corneum is maximal in cases where the thickness of the stratum corneum layer is more than the reduced scattering length. In the visible range of the spectrum, the light confinement phenomenon is maximal in stratum corneum layers with a thickness of at least 150μm (the blue range) and 600 m (the red range). In addition, the relative effect of light confinement increases with the decrease of the underlying tissue reflectance. If unaccounted for, the stratum corneum light confinement (SCLC) phenomenon may potentially lead to an inaccurate estimation of the light distribution, resulting in errors in some skin diagnostic parameters measured via the diffuse reflection, such as water and total hemoglobin content and blood oxygenation.

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