Modelling Skin Diffuse Reflectance Spectra in the Near-infrared Spectral Range

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INTRODUCTION

Monte Carlo method was used in this study to simulate diffuse reflectance spectra of the human skin to better understand the optical properties of the human tissue in the near-infrared wavelength range. By comparing the simulation spectra to experimentally taken spectra, we can estimate the relative volume fractions of different chromophores that have distinct absorption spectra in this wavelength range (water, lipids, collagen and elastin). The normalised absorption coefficient values are displayed in Figure 1.

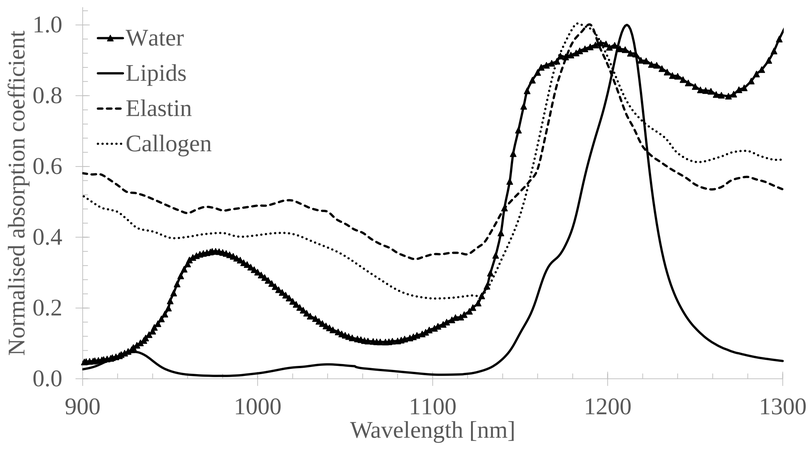

Figure 1 Normalised absorption coefficient values of different chromophores inside human tissue[1-3].

A *Matlab* based graphical user interface was created for faster spectral analysis and spectra comparison with the ability to set different optical parameters of the tissue model for the simulation program input and read the output of Monte Carlo simulation programs like *MCML* - Monte Carlo for Multi-Layered media, created by *Wang and Jacques (1995)*[4].

METHODS

Optical properties of each layer were described by the absorption coefficient $\mu_a(\lambda)$, scattering coefficient $\mu_s(\lambda)$, refractive index n and anisotropy factor g. Layer thickness d was also specified, so all the necessary parameters for *MCML* input are defined. The absorption coefficient $\mu_a(\lambda)$ for each layer was calculated by multiplying the absorption coefficient[1-3] of each chromophore with the respective volume fraction V of the chromophore:

$$\mu_a(\lambda) = \begin{bmatrix} \mu_{H_2O}(\lambda) \cdot V_{H_2O} + \mu_{lip}(\lambda) \cdot V_{lip} + \\ +\mu_{col}(\lambda) \cdot V_{col} + \mu_{ela}(\lambda) \cdot V_{ela} \end{bmatrix} cm^{-1}$$

The reduced scattering coefficient $\mu_s'(\lambda)$ was calculated according to Mie and Rayleigh scattering theory as proposed in previous studies[5]:

$$\mu_s'(\lambda) = [1.1 \cdot 10^{12} \cdot \lambda^{-4} + 73.7 \cdot \lambda^{-0.22}]\ cm^{-1}$$

The anisotropy factor g is introduced to calculate the full scattering coefficient for μ_s for each layer[4]:

$$\mu_s(\lambda) = k \cdot \frac{\mu_s'(\lambda)}{1-g}\ cm^{-1}$$

Multiple test simulations were performed to better understand how each optical property (absorption coefficient, scattering coefficient, refractive index, etc.) affects the simulated spectra. For this, a three-layer model was constructed based on optical parameters that have been discussed in previous studies[4-9] for healthy human skin on the forearm. Collagen and elastin volume fractions are specified by the remaining volume after water and lipid fractions are applied. The parameters used for this model are displayed in Table 1.

Parameter	Stratum Corneum	Epidermis	Dermis
V_{H_2O}	0.30	0.65	0.65
V_{lip}	0.05	0.05	0.10
V_{col}	0.40	0.18	0.15
V_{ela}	0.25	0.12	0.10
$d, \mu m$	20	80	2000
g	0.86	0.80	0.90
n	1.50	1.35	1.40

Table 1 Tissue model for MC simulations. $V_{H_2O}, V_{lip}, V_{col}, V_{ela}$ – respective volume fractions of water, lipids, collagen, elastin; d [μm] – layer thickness; g – anisotropy factor; n – refractive index.

RESULTS

Some examples of the simulations performed to analyze different optical parameter changes on the resulting spectra are displayed in Figure 2 and 3. Changes in volume fractions of different chromophores left an unique fingerprint on the resulting diffuse reflectance (DR) spectrum, which lets us identify these chromophores when analyzing experimentally taken DR spectra.

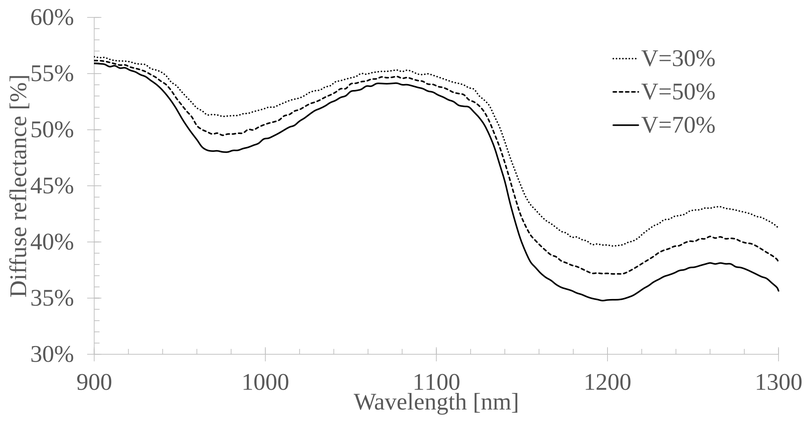

Figure 2 Diffuse reflectance spectra of changes in volume fraction of water V_{H_2O} in the epidermis layer.

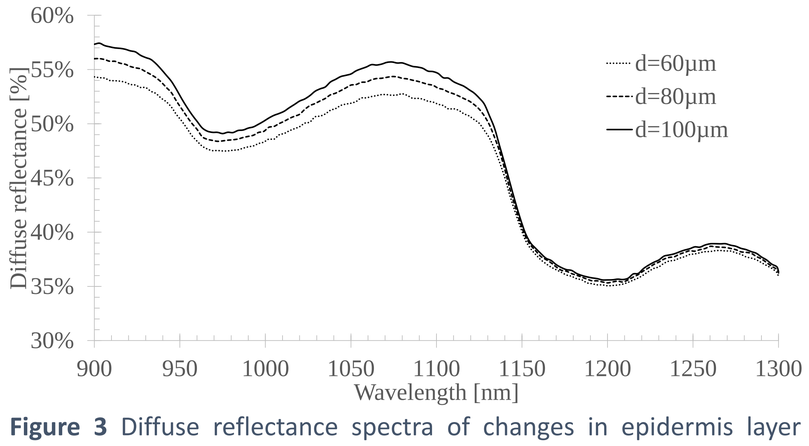

Figure 3 Diffuse reflectance spectra of changes in epidermis layer thickness d.

It was also observed that some parameter changes affect the simulated spectra quite similarly. This can potentially lead to problems revolving around identical spectra on different changes being made to several parameters (Figure 4). This can lead to a potential error in the attempts to determine exact or relativistic volume fractions of different chromophores in human skin when trying to examine experimentally taken absorption spectra.

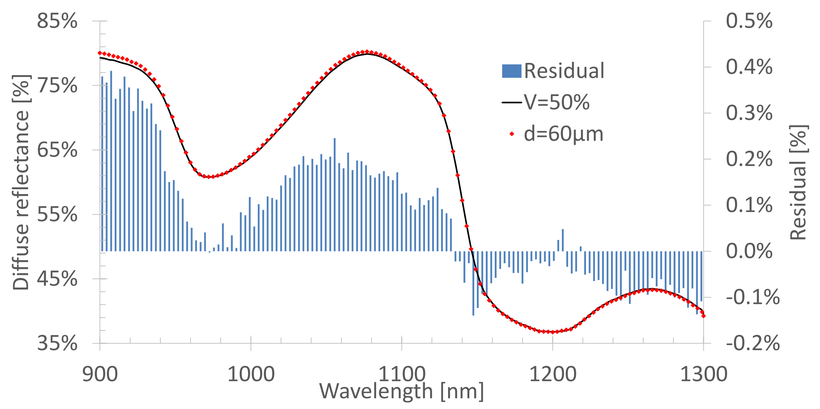

Figure 4 Comparison between the simulated DR spectra with changes made to epidermis layer thicness ($d = 60\ \mu m$ case) and volume fraction of water ($V_{H_2O} = 50\%$ case). Secondary axis – residual values.

Taking all this gathered information in account, several experimentally takes spectra were analyzed with the spectral overlapping method. One example is shown in Figure 5.

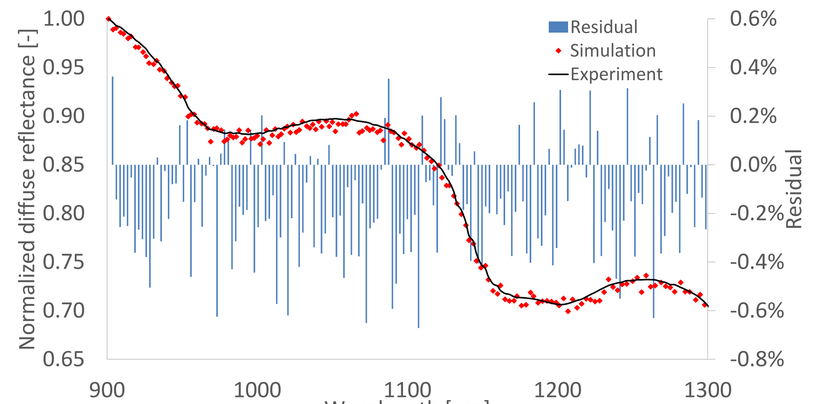

Figure 4 Comparison between an experimentally taken DR spectrum from normal forearm and simulated spectrum using inverse Monte Carlo approach. Secondary axis – residual values. Water volume fraction was estimated to be 0.38 in the Stratum Corneum, 0.68 in the Epidermis layer. Stratum Corneum layer thickness was determined to be 25 μm and epidermis layer thickness - 105 μm.

CONCLUSIONS

1. It is possible to identify NIR absorbing chromophores in DR spectra, as each of them leaves a unique fingerprint on the spectra;
2. There is potential for non-invasive approximation of different optical properties of human tissue by an inverse Monte Carlo approach if some parameters of the tissue are already known.

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