Modeling diffuse reflectance spectrum of skin in the near-infrared spectral range by Monte Carlo simulations

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Introduction

Diffuse reflectance spectroscopy can be a powerful tool for understanding the optical properties of human tissue, but by looking at a spectrum alone will not allow one to make use of the information caintained within.

By making use of the forward Monte Carlo (MC) method you can effectively simulate light interaction with tissue, and by changing the optical properties of your tissue model, you can notice changes in the diffuse reflectance spectrum that you get out of the simulation. Analysing these changes in the spectrum from the model can then allow you to make assumptions of the optical properties of *in vivo* diffuse reflectance measuements.

Model

First , a model to represent real human tissue needs to be created. A seven layer model was created using slightly modified data from *Meglinski and Matcher (2003)*[1] and *Kim et al* (2012)[2]. All the values used with this model are represented in Table 1.

The absorbtion coefficient μ_a for all layers (except LE) was calculated:

$$\mu_a(\lambda) = \mu_{H_2O}(\lambda)C_{H_2O}(1 - \gamma C_{blood}) + \mu_a^0(\lambda)(1 - \gamma C_{blood})(1 - C_{H_2O}) \quad (1)$$

The wavelength range used was the near infrared range of 900 nm to 1700 nm. Melanin presence was taken in concideration for the Living epidermis layer:

$$\mu_a^{LE} = [C_{mel}\mu_a^{mel} + (1 - C_{mel})\mu_a^0](1 - C_{H_2O}) + C_{H_2O}\mu_{H_2O} \quad (2)$$

where μ_a^{mel} based on *Jacques and McAuliffe (1991)*[4] is given:

$$\mu_a^{mel} = 1.7 \times 10^{11}\lambda^{-3.48} \, [mm^{-1}] \quad (3)$$

Methods

The MC simulations were done using the code provided by *Wang et al. (1995)*[3]. The MC simulations need the following input parameters for each layer – absorbtion coefficient, scattering coefficient, anisotropy, layer depth and refractive index. As a medium above the layers there was air (n=1) for all simulations. Number of photon packets also need to be specified – for all simulations there were 10^6 photon packets used, that enter the model from above at the air-stratum corneum boundary with the starting photon weight W of 1. At this point a set probability determines if the packet gets reflected speculary or it enters the tissue. When a packet has entered the tissue, it can be partially or fully absorbed by uniformly distributed bins throughout the tissue. Every time a packet interacts with a bin it loses part of its weight and then gets scattered in a different direction determined by the anisotropy factor and scattering coefficient. After a photon looses a specified amount of its weight (in this case if $W = 0.001W_0$) it gets completely absorbed and the next photon packet starts entering the tissue. At the end of the simulation, when the last photon packet gets terminated, all absorbed and diffusely scattered weight of the photons gets added up to create a absorbtion and reflectance probability.

Results

To fully explore the capabilities of this model, there were made 52 different sets of input parameters for the ranges of data listed within Table 1. The wavelength range was divided in 250 different points and to each point there was a different absorbtion coefficient specified, so 13000 simulations were made. The results show that the most changes to the spectrum were made by the water and melanin concentrations of Living epidermis layer and water concentrations of the Reticular dermis layer as shown in Figure 1, Figure 2 and Figure 3.

Figure 1. LE water concentration

Figure 2. LE melanin concentration

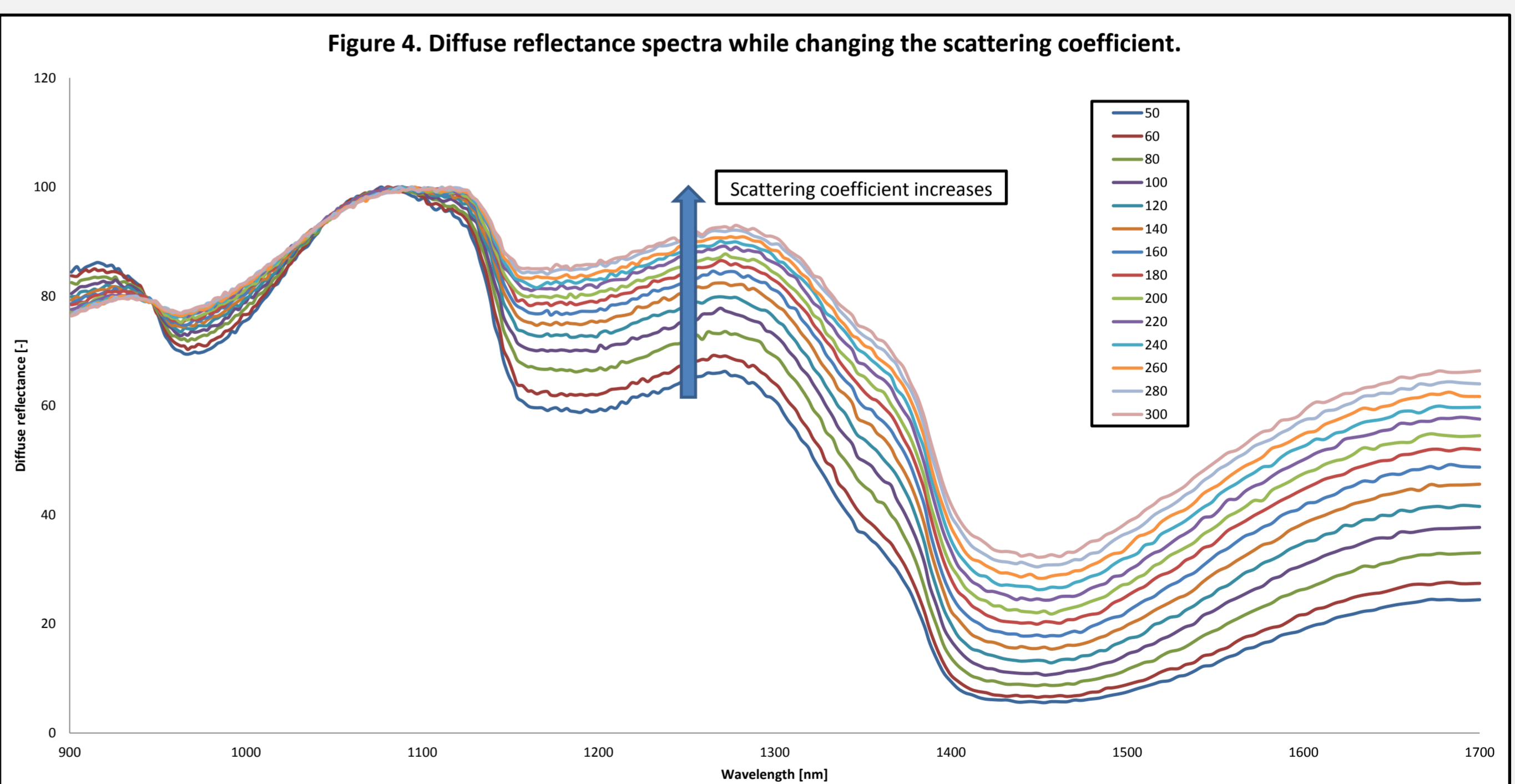Figure 3. RD water concentration
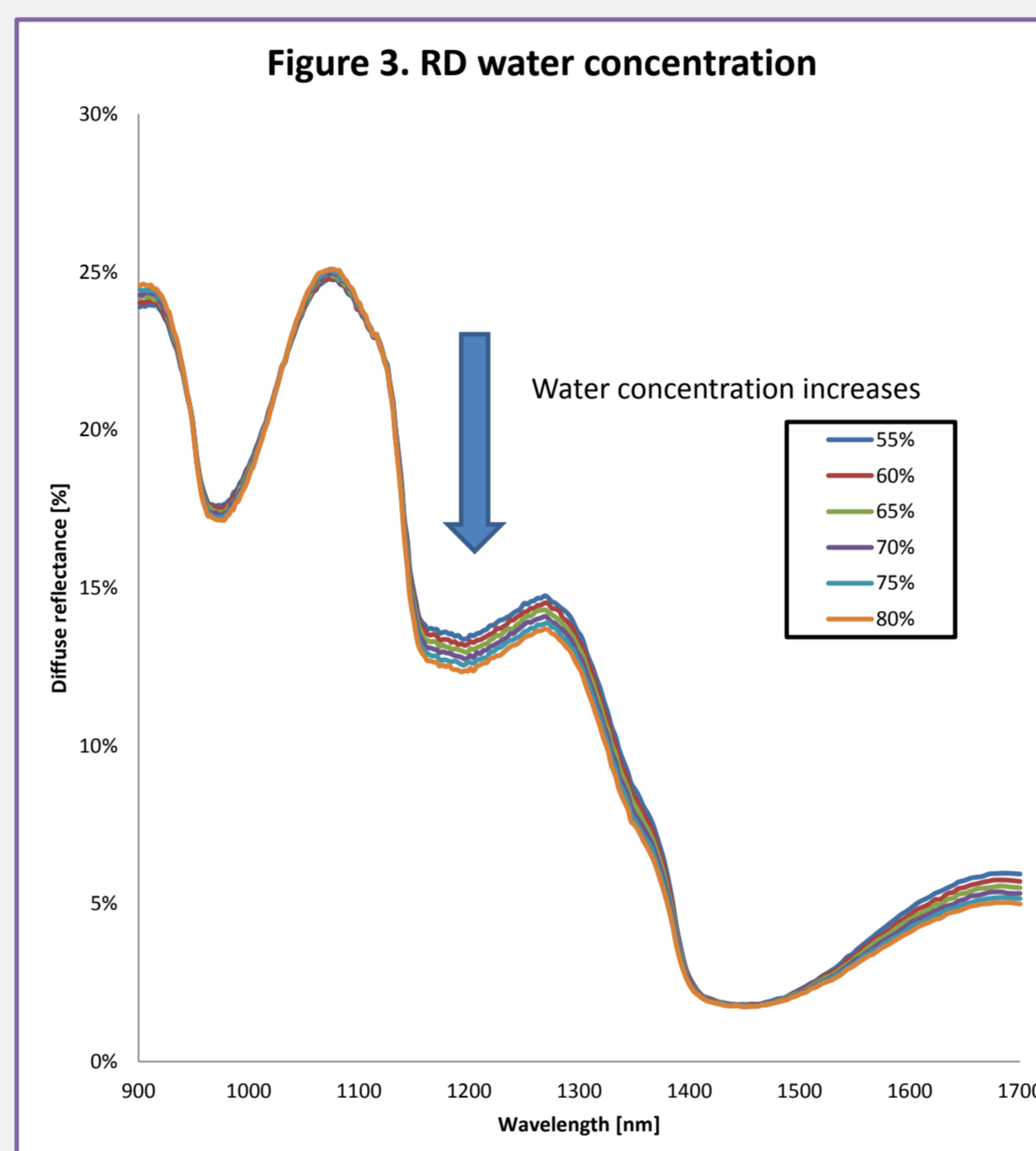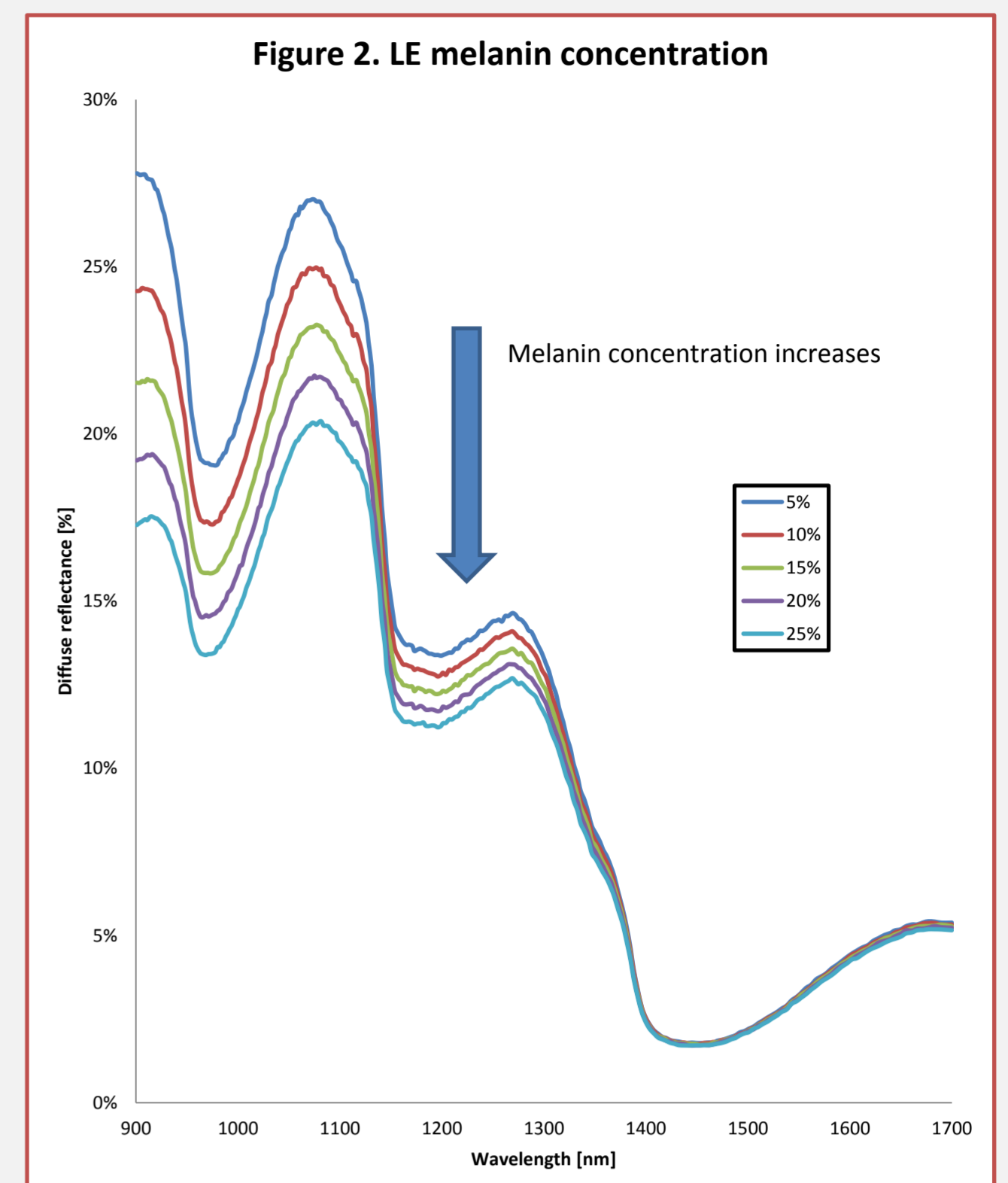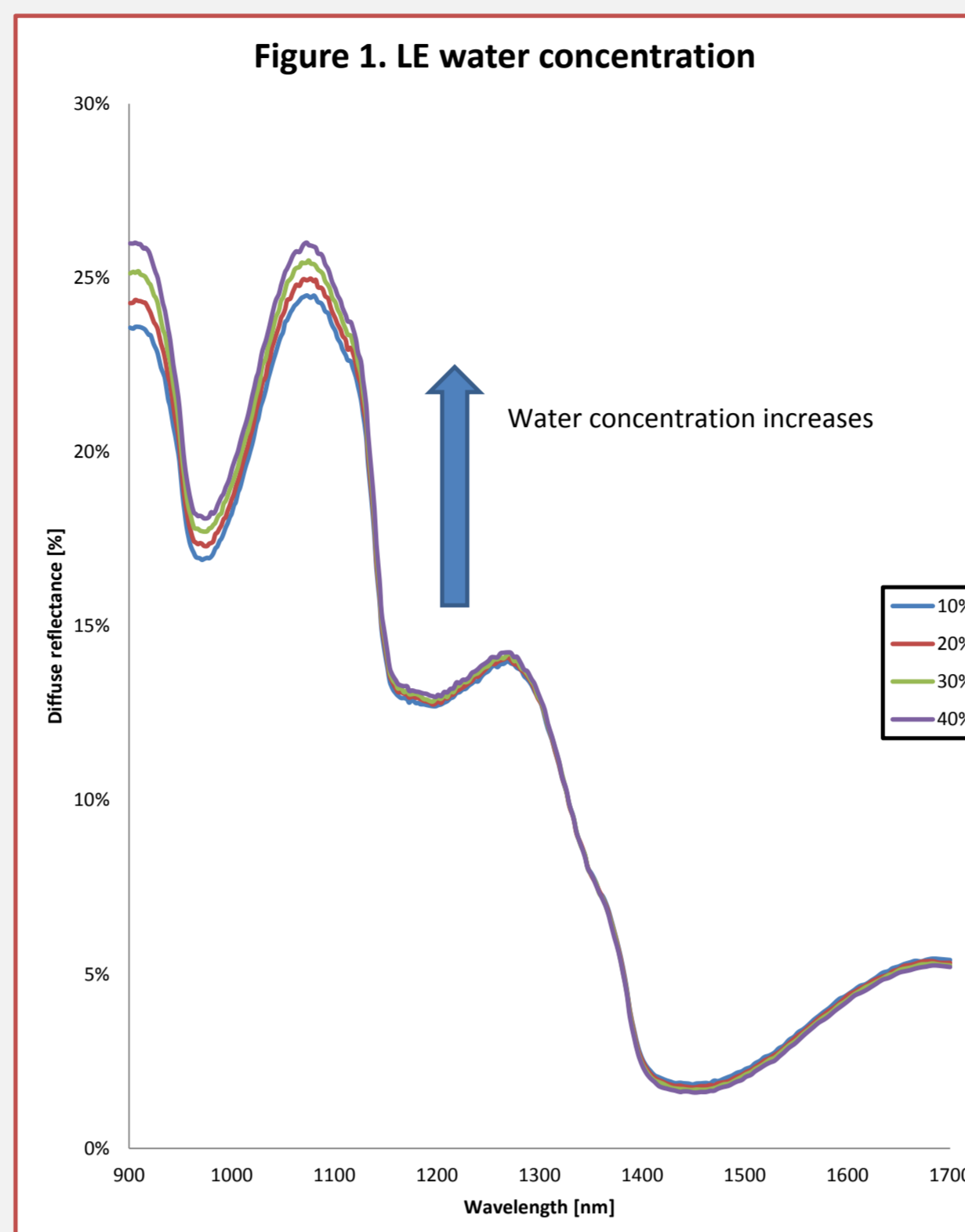
Results

There was also a model created in which the melanin concentration was set to 5% and all the other input parameters remained constant except for the scattering coefficient. Values of 50 to 300 cm^{-1} were used for the scattering coefficient equal to all layers. The results can be seen in Figure 4.

Conclusions

The seven layer human tissue model discussed in this study has proven to be useful for determening the optical properties by analysing the diffuse reflectance spectre. You can clearly see the spectrum change if there are different concentrations of water and melanin in the skin. It was also revealed that the change of the scattering coefficient changes the spectrum even more.

By using these results of the simulations, you could effectively compare them to experimentally measured *in vivo* diffuse reflectance specta with an inverse MC approach and determine the scattering coefficient of the measured tissue.

Figure 4. Diffuse reflectance spectra while changing the scattering coefficient.

Layer	S	C_{water}	C_{mel}	C_{blood}	γ	d [μm]	g	n	μ_s [cm^{-1}]
Stratum corneum	0	0.05-0.5	0	0	0	1-4	0.86	1.5	100
Living epidermis	0	0.1-0.4	0.05-0.25	0	0	80-100	0.8	1.34	45
Papilary dermis	0.6	0.4-0.6	0	0.03-0.06	0.099	15-20	0.9	1.4	30
Upper blood net dermis	0.6	0.5-0.7	0	0.3	0.111	8-10	0.95	1.39	35
Reticular dermis	0.6	0.55-0.8	0	0.05	0.111	140-160	0.8	1.4	25
Deep blood net dermis	0.6	0.6-0.8	0	0.14	0.124	8-12	0.95	1.38	30
Subcutaneous Fat	0.6	0.6	0	0.06	0.111	800	0.75	1.44	5

Table 1. Optical properties of the human skin model. S – oxygen saturation, C_{water}, C_{mel}, C_{blood} – volume concentrations of water, melanin, blood, d – depth, g – anisotropy, n – refractive index, μ_s – scattering coefficient.

Literature
[1]Computer simulation of skin reflectance spectra (Meglinski and Matcher, 2003)
[2]Reflectance spectroscopy of normal and bruised human skins: experiments and modeling (Oleg Kim *et al.*, 2012)
[3]Monte Carlo Modeling of Light Transport in Multi-layered Tissues in Standart C (Wang *et al.*, 1995)
[4] The melanosome: threshold temperature for explosive vaporization and internal absorption coefficient during pulsed laser irradiation (Jacques S. L. and McAuliffe D. J., 1991)

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