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DOI:
https://doi.org/10.1117/12.3001853

Document Version
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Citation for published version (APA):
Bahl, A., Segaud, S., Xie, Y., Shapey, J., Bergholt, M., & Vercauteren, T. (2024). A comparative study of analytical tissue reflectance models using simulated and experimental data. In A. Wax, & V. Backman (Eds.), *Biomedical Applications of Light Scattering XIV* (Vol. 12856, pp. 1285608). Article 1285608 (Progress in Biomedical Optics and Imaging - Proceedings of SPIE; Vol. 12856). SPIE. https://doi.org/10.1117/12.3001853

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Download date: 17. Jun. 2024

A comparative study of analytical tissue reflectance models using simulated and experimental data

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1. INTRODUCTION

Three major one layer tissue models (Modified Beer-Lambert,[1] Jacques 1999,[2] Pilon 2009[3]) are compared to Monte Carlo simulated diffuse reflectance spectra and measured tissue phantom spectra with known ground truth. These ground truth values were obtained using inverse adding doubling and absorbance measurements and validated using a phantom with known ground truth (BioPixs). Finally, a two layer model (Pilon 2009) was evaluated against Monte Carlo simulations and used to analyse skin reflectance data (NIST[4]). These models were compared on goodness of fit and parameter extraction accuracy.

It was found that the Pilon 2009 one layer model performed best against Monte Carlo simulations and phantom measurements, however the Pilon 2009 two layer model had significant regions of inaccuracy. These inaccurate regions correspond to circumstances where the epidermal layer has significant thickness and melanin content, while the dermal layer has low fraction of blood meaning that the haemoglobin impact is “masked”. The extraction of parameters from the NIST skin dataset using this model returns values that do not correspond well to literature values suggesting that many of these spectra lie within an inaccurate region or indicates oversimplification of the tissue modelling. This suggests both Pilon 2009 and Jacques 1999 are suitable for modelling tissue that can be approximated as a single, homogeneous, semi-infinite slab, however the Pilon 2009 two layer model is not yet effective when encountering empirical data.

2. METHODS

2.1 Modelling optical properties

All three reflectance models ($R(\lambda)$) utilise absorption (μ_a) and reduced scattering (μ_s') parameters as inputs which must be modelled for tissue. We take the Yudovsky dermis absorption coefficient to model the semi-infinite tissue slab as well as the dermal layer in the double-layer configuration.[3] We also use the Yudovsky epidermis absorption coefficient to model the absorption of the epidermal layer in the double-layer configuration.[3] Finally, we use the Jacques Mie scattering equation to model the reduced scattering coefficient for all scenarios,[5] where the dermal and epidermal layers share a single reduced scattering coefficient as in Yudovsky.[3]

The Jacques single-layer model is applied as in the original publication,[2] however we use our own hyperparameters which we obtain by fitting to a Monte Carlo dataset. The Yudovsky single-layer model is applied using the simplified formulation in their Erratum publication.[6] We also utilise the original Yudovsky double-layer model alongside this single-layer formulation.[3] The Modified Beer-Lambert single-layer model has a variety of formulations.[1,7] We thus allow for further flexibility in this model by introducing linear scaling hyperparameters (M_{1-3}) that we fit to a Monte Carlo dataset: $R(\lambda) = \exp\left(-\frac{A(\lambda)}{100}\right)$ where $A(\lambda) = M_1\mu_a(\lambda) + M_2\mu_s'(\lambda) + M_3$.

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Biomedical Applications of Light Scattering XIV, edited by Adam Wax, Vadim Backman,
Proc. of SPIE Vol. 12856, 1285608 · © 2024 SPIE
1605-7422 · doi: 10.1117/12.3001853

We generate a Monte Carlo simulated two datasets of 100 diffuse reflectance spectra each with refractive index of 1.44 to mimic biological tissue. The first of these models a single semi-infinite slab, whereas the second models a two-layer geometry mimicking skin. We also synthesise gelatin-based optical tissue-mimicking phantoms using Acid Red 1 (AR1, 210633, Merck, Germany), Acid Red 14 (AR14, B22328, Fisher Scientific, England), and Intralipid and measured using a dual-beam integrating sphere PerkinElmer Lambda 750s spectrophotometer. Finally, a NIST total reflectance dataset measured from the forearms of 100 healthy volunteers using an integrating sphere spectrophotometer[4] is used to evaluate the double-layer model, however this is not associated with ground truth parameters.

The quality of the forwards models using ground truth parameters to predict reflectance spectra is evaluated using Normalised Root Mean Squared Error ($NRMSE$) whereas the inverse problem solutions are evaluated using the absolute percentage errors between the fitted and ground truth parameters.

3. RESULTS

3.1 Single-layer models

Table 1 shows the $NRMSE$ for the diffuse reflectance spectra generated by the forwards single-layer models compared to the Monte Carlo simulated spectra or the measured phantom spectra. This demonstrates that Yudovsky 2009 provides the best spectral reconstruction performance, followed closely by Jacques 1999. It also shows a poorer performance of these models when modelling measured spectra compared to simulated spectra.

Table 1: Mean (standard deviation) $NRMSE$ (3.d.p.) between each forwards spectrum from each model and each of Monte Carlo simulated spectrum or measured phantom spectrum using the same ground truth variable parameters for each analytical model evaluated for the wavelength region of 450-600nm. These are presented alongside the median (inter-quartile range) Absolute Percentage Error (APE) of the StO_2 parameter extracted from Monte Carlo simulated spectra and the $AR1$ parameter extracted from the measured phantom spectra.

Model	$NRMSE$		APE (%)	
	Simulated	Measured	StO_2	$AR1$
Yudovsky 2009	0.013 (0.006)	0.059 (0.031)	0.913 (1.92)	1.59 (11.0)
Jacques 1999	0.037 (0.065)	0.075 (0.032)	2.21 (4.97)	7.02 (20.2)
Modified Beer-Lambert	0.630 (0.461)	0.464 (0.294)	43.0 (49.8)	83.5 (57.0)

Table 1 also shows examples of the quality of parameter extraction using the inverse problems to analyse Monte Carlo simulated data (to extract StO_2) and measured phantom spectra (to extract $AR1$). These also show Yudovsky 2009 performing best closely followed by Jacques 1999 with the performance quality reducing when used to analyse measured spectra compared to simulations.

3.2 Double-layer models

The forwards double-layer Yudovsky 2009 model is evaluated against Monte Carlo simulated diffuse reflectance spectra. A mean (± standard deviation) $NRMSE$ of 0.167(± 0.133) demonstrates considerable variability in the quality of fit. This analysis is not possible when considering the measured NIST dataset due to the lack of known ground truth.

The Monte Carlo simulated dataset is analysed using the inverse problem corresponding to the double-layer Yudovsky 2009 model. This resulted in a mean (± standard deviation) absolute percentage error for the extracted StO_2 of 15.3% (± 27.5%) demonstrating considerable variability in the parameter extraction. Ten Monte Carlo diffuse reflectance spectra are simulated where the StO_2 is varied between 0 and 100% and scattering parameters are fixed. The Yudovsky two layer model is fitted by least squares to each of these Monte Carlo spectra and a linear regression is fitted between the extracted and input StO_2. The r value is then plotted in the remaining 3D parameter space (f_{blood}, f_{mel}, L_1) and coloured by value which is shown in Figure 1. This shows that the effect of StO_2 on the diffuse reflectance spectrum is masked by the melanin effect in areas of low f_{blood}, or high L_1 or f_{mel} leading to poor StO_2 extraction in these areas.

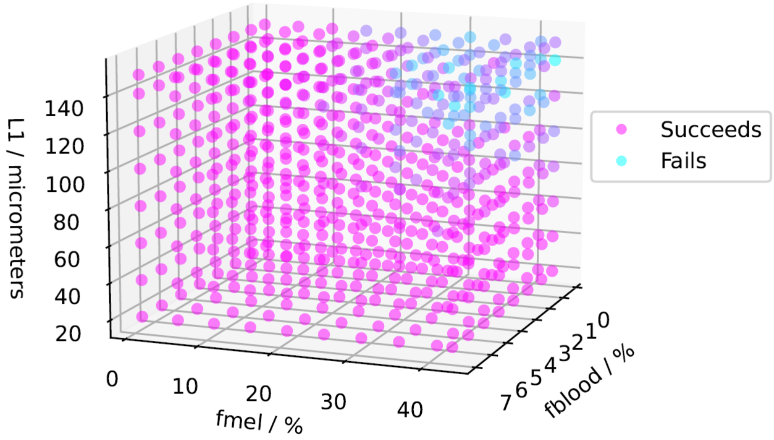

Figure 1: A depiction of the impact of 3 key physiological parameters ($L1$ being thickness of the epidermal layer, $fmel$ being volume fraction of melanin in the epidermal layer, and $fblood$ being volume fraction of blood in the dermal layer) on success of StO_2 extraction by Yudovsky 2009 double-layer model. Here success is determined by the Pearson correlation coefficient (r) between extracted and ground truth StO_2 of 10 Monte Carlo simulations using the designated combination of physiological parameters. r is mapped by colour where the key shows the extremes of this scale where r=0.988 (highly successful) or r=-0.683 (failure).

The measured NIST skin dataset is analysed using the inverse problem of the Yudovsky 2009 double-layer model, which results in a mean (± standard deviation) extracted StO_2 of 39.6% (± 11.1%). This shows significantly different results from previous literature analysis, such as 78.3% (± 12.9%)[8] or 71% (± 16),[9] suggesting that this model should be used with caution when encountering experimental data.

4. DISCUSSION

When compared to Monte Carlo simulations or measured phantom spectra, the semi-empirical Yudovsky model performs best in terms of fit and parameter extraction, followed closely by the Jacques model.

Whilst the Yudovsky single-layer model has excellent spectral prediction,[10] this quality cannot be fully replicated by the Yudovsky double-layer model. The weaknesses of this model were shown to be in regions of high L_1, high f_{mel}, and low f_{blood}. Consequently, in regions of epidermis where the impact of melanin is significant, it "masks" low haemoglobin impact from the dermis. For this reason, this model should be used with caution as it has limited use in the regions of failure identified. When fitting to NIST skin experimental data, the parameters returned are largely different to previous literature values for healthy individuals, suggesting that these data may lie in the failure region of parameter space, or that a simple two layer model may be too crude an approximation.

In conclusion, the Yudovsky single layer model works well for modelling of tissue that can be approximated by a semi-infinite, homogeneous slab. Jacques is also able to well approximate this with a simpler model. The double-layer Yudovsky model, however, does not perform with the same quality as the single-layer model and has some clear failure regions, demonstrating that this model should be used with caution.

Acknowledgements. This project is funded by the NIHR [NIHR202114]. The views expressed are those of the author(s) and not necessarily those of the NIHR or the Department of Health and Social Care. This work was supported by core funding from the Wellcome/EPSRC [WT203148/Z/16/Z; NS/A000049/1]. TV is supported by a Medtronic / RAEng Research Chair [RCSRF1819\7\34]. TV and JS are co-founders and shareholders of Hypervision Surgical Ltd, London, UK. For the purpose of open access, the authors have applied a CC BY public copyright licence to any Author Accepted Manuscript version arising from this submission.

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