Simulation study of the quantitative prediction of oleic acid concentrations by near infrared spectroscopy in pig carcasses

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Introduction

In situ analysis through skin is crucial for in-field and online use of near infrared (NIR) spectroscopy in the livestock industry, owing to the ease and speed of spectra collection. Pérez-Marín et al.[1] demonstrated the capacity for NIR spectroscopy to quantitatively predict fatty acid profiles in live pigs, although the models showed lower accuracy compared to intact subcutaneous adipose tissue analysis. Reduced accuracy could be partly explained by light attenuation as it travelled through skin. Knowing how sensitive measurements through skin are to changes in the fatty acid profile of the hypodermis is important for understanding light-tissue interactions. The purposes of this study were to investigate changes in NIR spectra caused by oleic acid (OA) concentration in the hypodermis layer, to simulate measurements through the full pig skin, and to predict OA concentration by applying multivariate analyses.

Materials and Methods

A Monte Carlo method was used for simulating absorbance spectra through pig skin. This method has been widely used for strongly scattering media such as human skin tissue.[2] Different input parameters were required, including refractive indices and the optical properties and thicknesses of each layer. Refractive indices (n) of porcine epidermis were reported by Ding et al.[3] for single wavelengths between 325 nm and 1557 nm; for dermis and subcutaneous adipose tissues n was fixed at 1.36. Pig skin optical properties have been studied by Du et al.[4] for dermis in the 900–1500 nm range and by Cain et al.[5] in the 1000–1600 nm range for epidermis and dermis (i.e. providing the absorption coefficient (μ_a), the scattering coefficient (μ_s) and the anisotropy parameter (g)). For subcutaneous adipose tissue, rat data reported by Bashkatov et al. [6] were used as no data were found for pig hypodermis. The thicknesses used in the simulation for each layer were reported by Renaudeau et al.[7] The wavelength range studied was 1100–1300 nm. The effect of the oleic acid concentration was only estimated based on changes on the absorption coefficient for the hypodermis, since it was assumed that the size, shape and refractive index of the scattering particles do not change. The reflectance spectra of the pig skin were simulated by varying the absorption coefficient of the hypodermis from 0 to 2 cm^{-1}. Values of μ_a calculated for OA concentrations ranging from 30 to 70% were based on μ_a values reported for 50% oleic acid in pig fat (in the range 1100–1300 nm).[8] The reflectance value for each wavelength from the simulated results was subsequently estimated by regression for each μ_a and each OA concentration. As Monte Carlo simulation is a statistical method, a large number of photons are desirable to obtain reliable results. In our case, 1,000,000 photons were launched. The differences found in the simulated absorbance spectra were transferred to spectra measured from pig skin with a Foss NIRSystems spectrometer, and were applied to average spectra from 20 pigs with different OA concentrations in adipose tissue. Modified partial least squares (MPLS) regression was tested for the prediction of OA.

Results and Discussion

Changes in the reflectance spectra for each wavelength were simulated for different absorption coefficients in the hypodermis layer. Other parameters (i.e. refractive index, optical properties and thickness of the different layers) were held constant. Figure 1 shows the simulated changes in absorbance (log (1/reflectance)) at 1200 nm (i.e. lipid absorption band)[9] for different μ_a values. Larger absorbances correspond to larger absorption coefficients, with a slightly stable tendency for values above 1 cm^{-1}, Here, this stable tendency was observed at the other wavelengths evaluated (i.e. 1100–1300 nm).

Simulated absorbance values were used to estimate spectra at different OA percentages. Estimates of μ_a for different OA concentrations (from 30% to 70%) were based on μ_a values for 50% OA in pig fat; the corresponding absorbances were estimated by regression. Figure 2 shows the simulated results of reflectance spectra for different concentrations of OA in the pig hypodermis. The absorbance increased at all

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wavelengths with increased OA concentrations; hence, changes in spectra may be too small to be accurately predicted with multivariate analysis methods.

The simulated absorbance spectra (Figure 2) were processed with MPLS regression. The calibration models obtained for the prediction of oleic acid concentration are shown in Table 1. A second derivative provided better statistics for this parameter. The coefficient of determination of cross-validation (R^2_{CV}) was above 0.99; this value was indicative of the variability explained by the model accuracy. The standard error of cross-validation (SECV) displayed a value of 0.89%. This indicates the possibility of predicting different oleic acid concentrations for NIR spectroscopic measurements performed through pig carcass skin.

Pérez-Marín et al.[1] obtained predictive models for oleic acid concentration using NIR spectroscopic measurements taken through the skin of Iberian pig carcasses. They reported a SECV of 1.48% and R^2_{CV} of 0.80 for measurements at the slaughter house (with a LabSpecPro A108310 Analytical Spectral Device-ASD; 400–2000 nm), while a SECV of 1.44% and R^2_{CV} of 0.82 for measurements performed at the laboratory (Foss NIRSystems 6500, 450–2300 nm). These errors are larger than those reported here with simulated spectra, but it should be remarked that some assumptions have been considered to perform the simulation.

Clear differences were observed between measured and simulated pig skin spectra due to the simplifications considered, such as instrumental design, scattering changes due to different OA, absorbance is not referred to the number of caputred photons, etc. Changes due to different OA concentrations in measured spectra were modelled to solve these differences. Figure 3 shows the spectra of several pig skins with different OA concentrations. These spectra were calculated from 1) the average spectra measured on the Foss NIRSsystems 6500 and 2) the differences for each wavelength simulated due to the changes on OA concentration in the hypodermis. Small changes in the absorbance spectra were also observed as in the case of simulated results. MPLS models were calculated with this new dataset (Table 2), and a second derivative reported a R^2_{CV} of 0.99 and SECV of 1.06%. The increase in SECV values as compared between simulated and measured spectra can be due to the physico-chemical complexity of the measured pig skin sample.

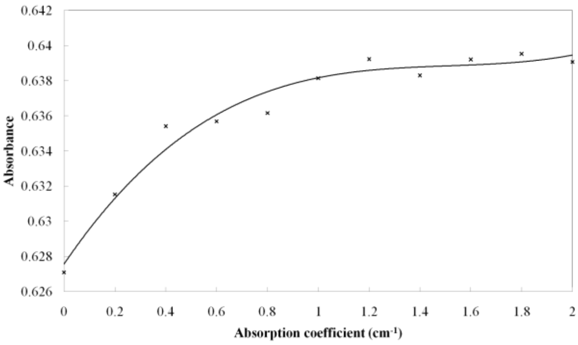

Figure 1. Estimated absorbance for different absorption coefficients of the hypodermis layer at the 1200 nm.

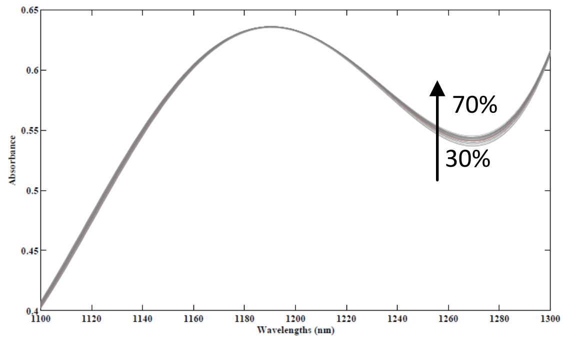

Figure 2. Spectra simulated with changes in oleic acid concentration in the adipose layer.

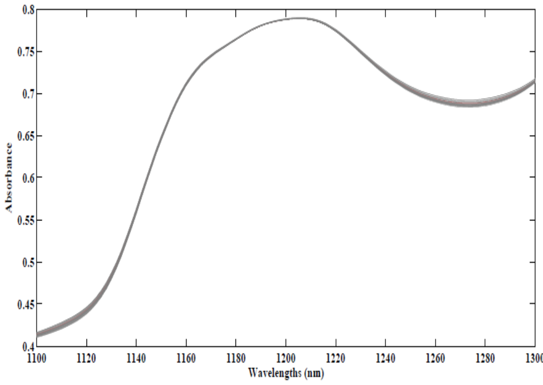

Figure 3. Estimated absorbance spectra measured through skin for pig carcasses with different oleic acid concentrations.

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Table 1. PLS models for the prediction of oleic acid concentration with simulated spectra and measured spectra.

Data	Pretreatment	No. samples	Latent variables	SEC (%)	SECV (%)	R^2
Simulated spectra	SNV+DT (2,5,5,1)	21	1	0.77	0.89	0.99
Measured spectra with the simulated changes in the spectra	SNV+DT (2,5,5,1)	21	1	0.96	1.06	0.99

Conclusion

The NIR reflectance spectra taken through the skin of pigs with different oleic acid concentrations in the hypodermis layer were simulated by a Monte Carlo method in the range 1100–1300 nm. This demonstrates mathematically and theoretically the possibility of detecting different oleic acid concentrations in subcutaneous pig adipose tissue with NIR spectroscopy, and the possibility of developing quantitative models for their prediction considering measurements through pig skin.

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