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Validated multi-wavelength simulations of light transport in healthy onion

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ABSTRACT

Multi-wavelength light transport simulations of individual brown onions have been validated in the wavelength range 710–850 nm by comparing the simulations with experimental results. The simulations used the Finite Element Method (FEM) implemented in the software code NIRFast in Matlab. NIRFast required tissue geometry, optical scattering and absorption properties as inputs. The scattering values were obtained from Inverse Adding Doubling (IAD) measurements of onion slices. The absorption properties of several components were investigated. They included water, chlorophyll and onion absorption values measured with the IAD method or using transmission measurements on onion juice. These inputs to NIRFast enabled simulations of the transmission through model onions with different light attenuation characteristics. Error between simulation and measurement was minimized using absorption values from onion juice. An imposed realistic water concentration constraint (~88%) removed cross talk between scattering and absorption. This resulted in a set of optical properties, based on a small set of component absorbers and Mie scattering theory, which accurately modelled light transport in each onion. The input absorption values were then checked for completeness with inverse simulations at each wavelength independently. Results indicated no major component was missing from the absorption model. The resulting optical property estimates were used to predict a range of transmission measurements from a high speed conveyor system.

1. Introduction and background

Near-Infrared (NIR) spectroscopy is a widely used method for non-destructively evaluating the qualities of produce in real time (Nicolaï et al., 2007). Commercial manufacturers of the NIR technology are continuing to look for new and improved technology. The development process could be significantly improved by having design and evaluation aided by computer software that estimates the interaction between light source, the produce being tested and the light sensors for any geometry. Several simulation methods exist already for modelling light propagation within biological tissue, the optical geometry and optical properties of the produce are the only components missing. Once developed, the software would allow virtual experiments to predict the wavelength dependent light attenuation through produce from potential NIR spectroscopic sensor designs.

Biological tissue is a highly scattering medium in the NIR range (approx. 700–1000 nm), where light is most likely to be scattered multiple times before experiencing an absorption event. Three main parameters are used to model transport in uniform biological tissue. The refractive index, n, determines the speed of light in the medium. The absorption coefficient, μ_a, determines how likely a photon is to be absorbed per unit distance and the reduced scattering coefficient, μ_s', determines how likely the photon is to have its travel direction completely randomized per unit distance. Light entering a highly scattering medium quickly scatters in all directions and takes many random short paths before being absorbed or exiting the medium. This process makes simulations the most practical method for predicting light propagation through highly scattering media, though theoretical calculations are possible in some simple cases (Martelli et al., 2009).

Two popular methods for simulating diffuse light transport are the Monte Carlo method and the Finite-Element Method (FEM). The Monte Carlo method simulates the trajectories of individual photon packets, indirectly solving the radiative transport equation (Martelli et al., 2009). This gives accurate results and is relatively easy to program, for example (Chugunov and Li, 2015; Fraser et al., 2003). A drawback is that, due to the scattering and absorption events, improving simulation accuracy away from the source requires an exponential increase in photon packets, and thus simulation time. This can be mitigated by using graphics processing hardware acceleration, for example Fang and Boas (2009) and Martinsen et al. (2009).

An alternative method is the FEM, which can be used to solve the light density diffusion equation, for example as implemented in the

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software NIRFast (Dehghani et al., 2008) for Matlab processing (Matlab, Natick, MA). This method simplifies the radiative transport equation by assuming the light transport is mostly isotropic. The equation of light transport then becomes a relatively simple diffusion equation (Martelli et al., 2009). The FEM is much more complicated to program and is not accurate close to the source due to the approximation of diffuse light propagation. In practice the benefit of the FEM is that it is much faster than the Monte-Carlo Method, generally by orders of magnitude in time, and that it yields accurate results away from the light source.

The inputs to these simulations include optical properties of the produce along with the shape of the produce and the locations of the light sources and detectors on the surface. Accurate inputs are needed to simulate realistic light transport in produce. Measuring the optical properties in biological tissue is often carried out using the Inverse Adding Doubling (IAD) method (Wang and Li, 2013; Wang et al., 2012). Another more expensive method is time-resolved reflectance spectroscopy (Cubeddu et al., 2001). Yet another method is the use of hyperspectral imaging combined with Monte Carlo simulations (Qin and Lu, 2009). One problem that arises is that these methods of measuring optical properties do not always agree (Saeys et al., 2008). Thus there are competing methods of measuring optical properties in the NIR range and some conflicting results from a variety of prior work.

The aim of this research was to validate FEM simulations with experiments, and to ensure the simulations generalize to new transmission geometries and onions. With this in mind we investigate the spectral region where we have observed light to be able to pass through the entirety of a medium onion, the so called biological window approximately 700–900 nm. In the following sections we report transmission experiments with precisely recorded geometry on three healthy onions. Following that is the validation simulations to recreate the transmission measurements using NIRFast. Finally, we compare simulations of a 180° transmission geometry with measurements on a high speed conveyor system for measuring NIR transmission spectra.

2. Simulation validation

The process for validating the simulations of light transport in onions was carried out in two main steps. The first was to collect the geometry of the experiment, the transmission readings from the experiment and absorption curves for major chromophores present in the onions. The second step was using these inputs to model a variety of possible optical properties for the onions, and selecting the optical property which simulated the real transmission measurements with the smallest error.

2.1. Collection of data for input to simulations

2.1.1. Optical properties estimates

Absorption coefficients of chemical components of the onion were gathered from various sources and in-house measurements. Fig. 1 shows the main absorption property estimates that were obtained. The first source was a plot of the chlorophyll absorption curve (Munns et al., 2016). The second source was from IAD method measurements on onion slices, completed in a previous study (Tomer et al., 2017). These prior measurements provided estimates of reduced scattering and absorption values. The absorption values are shown in Fig. 1, the reduced scattering values were parameterized using a heuristic Mie scattering formula required by NIRFast, (Fig. 1).

$$\mu_s'(\lambda) = SA * \lambda^{-SP} \quad (1)$$

SA is the scattering amplitude, SP is the scattering power, λ is wavelength of light in units of μm, and μ_s' is the reduced scattering coefficient. The IAD reduced scattering results from Tomer et al. (2017) indicated SP of 0.1 and SA from 11 cm^{-1} to 15 cm^{-1}. The measurement

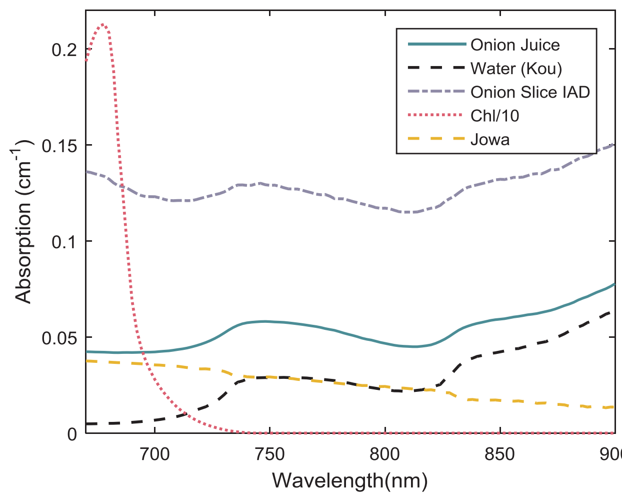

Fig. 1. Absorption curves used in simulations. The chlorophyll curve (Chl/10) is reduced by a factor of ten to fit on the graph. Jowa is the Onion Juice absorption minus Water absorption.

system used a single integrating sphere setup, and was validated using intralipid solutions at 0.5%, 1.0%, 1.5% and 2.0%, with worst case accuracies of 11% for scattering values, comparable to validation results published in literature. The physical setup used is described in detail in Rowe et al. (2014). An SP value of 0.1 was used in all cases in this study, while the scattering amplitude was initially 14 cm^{-1}. SA was later adjusted for improved simulations. The third source of optical properties was the water absorption curve measured by Kou et al. (1993). An absorption peak can be observed at 740 nm due to a 3rd overtone of OH-stretching, and the absorption peak near 840 nm is from a 2nd overtone O—H combination band (Golic et al., 2003). Finally a fourth source was obtained from transmission measurements on clarified onion juice, to provide a direct estimate for the absorption coefficient of onions without cross-talk with tissue scattering properties.

The absorption of onion juice was measured from tissue of two onions. The tissue samples were homogenized with a blender (Model 900, Nutribullet LLC, Pacoima, CA, USA). The homogenized sample was centrifuged at 3000 rpm for two minutes, which separated pulp from cloudy juice. The cloudy juice was then centrifuged at 10,000 rpm for 10 min at 2 °C, resulting in clear juice, effectively isolating the soluble solids with the water from the onion. The transmission setup was a 50 μm fibre from a broadband source connected to a collimator (F260 SMA-B, Thorlabs, Newton, NJ, USA) directing light through the sample to a second collimator (F260 SMA-B, Thorlabs, Newton, NJ, USA) which was coupled to a 400 μm fibre and a silicon spectrometer (MMS1, Zeiss, Oberkochen, Germany). The samples were held in a 40 mm fused silica cuvette.

Transmission measurements were made through the sample in a temperature controlled room at 21 °C. The effect from multiple reflections through the cuvette were calculated using a Markov chain model based on spectral refractive index values for fused silica (Malitson, 1965) and water (Daimon and Masumura, 2007). A Markov chain model is an alternative to theoretical calculations to predict the resulting transmission of reflections between four boundaries with index of refraction changes.

Light transmission through tap water was measured to evaluate the accuracy of the method. The water absorption values recreated the Kou absorption values to within a mean absolute error of 7%, and maximum error of 22%, in the range 710–850 nm. The Kou reference water absorption value at each wavelength was subtracted from the onion juice absorption value at each wavelength. This resulted in an effective "Juice omit Water Absorption" (Jowa) absorption curve, Fig. 1. This Jowa curve was used to add flexibility to the simulations. It allowed the combination of onion absorption and water absorption to vary from one