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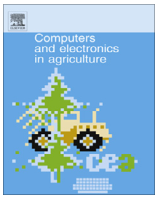

Monte Carlo simulation of light propagation in healthy and diseased onion bulbs with multiple layers

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ABSTRACT

It remains unanswered how the light interacts with healthy and pathogen-infected onion tissues in a multi-layer structure. The overall goal of this study was to simulate light propagation (including scattering and absorption) in healthy and pathogen-infected onion bulbs in the visible and near infrared (NIR) range using Monte Carlo simulations. Healthy onions and bulbs infected with two major onion post-harvest diseases, *Botritis Allii* (Neck Rot) and *Burkholderia Cepacia* (Sour Skin), were considered as the subjects of the simulation. Multi-layered models (18 layers in total) of healthy and infected onion bulbs were developed representing onion structure in the form of parallel slabs. Variance of optical properties was introduced into the models using median and quartile values computed from the experimental data. Monte Carlo-simulations were performed for the developed models to generate optical responses of 33 cases of healthy and infected onions representing different stages of disease propagation in the spectral range 550–1650 nm. Optical responses of all the cases were assessed with statistical tests. Study of spatially-resolved scattering reflectance was conducted to identify patterns typical for infected onions. Optical responses were measured experimentally to validate the simulation results for healthy onions. A total of 18 configurations (out of 33) of infected onions showed significant difference from healthy bulbs and demonstrated great potential for nondestructive detection. Confident detection was determined for onions with infection as deep as in the 3rd scale. The proposed optimal window for disease detection was 670–870 nm. The greatest discrepancy between optical response of infected and healthy onions was found at 800 nm. Spatially-resolved reflectance of the Neck Rot-infected onions showed consistent lower intensity than that of healthy onions over the entire studied radial range, whereas the Sour Skin-infected onions exhibited differences in a limited radial range. Light penetration simulation revealed that photons can reach 5–6 mm deep in the bulb in the case of one dry skin in the wavelength of around 800 nm and 1100 nm. Validation results suggested that although the overall pattern of the simulated results and experimental measurements was similar, the systematic error was likely caused by the curvature of the onion bulb and the measurement instrument. This study was the first attempt to use Monte Carlo simulations in the field of post-harvest research to model complex tissues of vegetables using more than 2 layers. The results of the simulation could be useful in developing non-destructive optical sensing methods for onions.

1. Introduction

There are more than twenty economically important *Allium* species in the world that are consumed in fresh and pickled form, as well as used for their distinctive flavor and color (Schwartz and Mohan, 2008). Among the *Allium* family, *Allium Cepa* (common onion) is the most commercially viable species with US production reaching over 7.3 billion pounds per year in 2010 (USDA, 2011a). Onion is the sixth largest vegetable crop in terms of annual per capita consumption, the fourth according to cash receipt, and the second in fresh market production in 2011 (USDA, 2011b).

To ensure quality, onion bulbs are mostly evaluated by human inspectors at the packing house, although machine vision methods are deployed in some large packing houses to evaluate onion size. In recent years, researchers have been trying to develop more advanced optical methods to evaluate both external and internal quality of onions. Feasibility of the optical approach for examining onion's physical properties was demonstrated by Birth et al. (1985) who investigated a spectroscopy method to non-destructively estimate the dry matter content in onion bulbs in the spectral range of 500–1200 nm. With the advancement of optical technologies and

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computing power, hyperspectral imaging was recently investigated in estimating dry matter content, solid soluble content, and firmness of onions in three optical configurations (Wang et al., 2013). The optical study of onions was advanced by Wang et al. (2012) who explored spatially-resolved reflection patterns in healthy and Sour Skin-infected onions in the range 950–1650 nm. The latest study conducted by the same group measured optical parameters of healthy and infected onion tissues both at a single wavelength (603 nm) and in a broad spectral range of 550–1650 nm (Wang and Li, 2013, 2014). Nicolai et al. (2007) presented multiple examples of successful applications of optical techniques in visible (VIS) and near-infrared (NIR) range to other vegetables and fruits, or biological tissues in general.

Understanding light behavior in complex tissues such as the multi-layered onion bulb is a key step towards development of an effective optical inspection system. Usually, light propagation in complex tissues is studied experimentally or modeled numerically. Experimental methods allow exploration of light patterns inside of fruits and vegetables with insertion of fiber optic probes at multiple locations within the object (Fraser et al., 2003). The experimental methods, however, are not only invasive and destructive, but also prone to errors due to multiple unnatural passages created in vegetables by removing certain part of the produce. Numerical modeling provides multiple advantages when studying complex biological tissues. It allows precise control over optical properties of tissue's structural components as well as provides easy access to any location within the tissue enabling possibilities for advanced analysis. Numerical modeling of light propagation in complex tissues typically relies on Monte Carlo-based algorithms. These algorithms are intended to solve radiative transfer equation for a large number of photon packets, handling each packet individually. Monte Carlo (MC) technique was successfully utilized to simulate steady-state (Wang et al., 1995) and transient (Boas et al., 2002) behavior of non-polarized and polarized (Ramella-Roman et al., 2005) light in complex geometries. In this study, a well-known Monte Carlo Multi-Layered package (MCML) was employed for simulations of the optical response in multi-layered onion tissues. A detailed description of this package is given in (Jacques, 2011; Wang et al., 1995). This tool was intensively tested in bio-optical studies in the field of bio-medical research. Gagnon et al. (2008) used MCML to simulate two-layered model of human head including brain tissue. Drakaki et al. (2008) employed this package to model spatially-resolved optical response in five-layered tissues representing porcine skin. Meglinski and Matcher (2003) applied MCML to model a seven-layered skin sample in the spectral range of 450–900 nm. Atencio et al. (2008) modeled a 3-layered neonatal skin with MCML in the spectral range of 400–700 nm. There were a few studies of using Monte Carlo simulation of light propagation in foods. For instance, Qin and Lu (2009) applied MCML for the study of semi-infinite one-layered apple fruit, Baranyai and Zude (2009) applied MCML to model one-layered kiwifruit, and Fraser et al. (2003) applied it for mandarin fruit also in one-layered configuration. Cen and Lu (2009) used two-layered model for validation of optical properties of optical phantoms in the spectral range of 500–1000 nm. Brázio et al. (2010) developed a simplified two-layer model using analytical methods to study spatially resolved reflectance in pears with a thin skin. So far, no studies have been reported to simulate photon interactions with complex multi-layered (more than two layers) tissues for fruits and vegetables.

In addition, the existing literature shows that most simulations were based on single input which did not take into account the variance of optical properties in biological samples. When conducting a case study, such simulations provided single values of optical response as the output for each case. Comparison of different cases becomes difficult due to the absence of a clear criterion that sets a threshold to differentiate significant and insignificant discrepancies in optical responses of studied cases. A few attempts have been made so far to include the variance of optical properties into MC simulations. Qin and Lu (2009) used four combinations of input parameters based on minimal and maximal values of optical properties measured for apple fruit. Baranyai and Zude (2009) implemented variability by selecting mean values of input parameters and introducing ±20% variation to these values. They used MCML in a single-layer configuration and employed the multi-factor ANOVA test to estimate the effect of input variation on optical responses generated with MCML.

In this study, the MCML package was utilized in conjunction with a convolution program (CONV) to assess optical responses of multi-layered onion tissues of healthy and pathogen-infected bulbs. Two major onion diseases, *Botritis Allii* (Neck Rot) and *Burkholderia Cepacia* (Sour Skin), were considered for simulation of infected bulbs. The overall goal of this study was to advance the understanding of spectrally and spatially-resolved optical responses of multi-layered onion bulbs with the presence of infection of two diseases at certain scales of bulbs using Monte Carlo simulations. Specific objectives were to: (1) simulate both the spectrally and spatially resolved scattering reflectance patterns for healthy, Neck Rot and Sour Skin infected onion bulbs with various infection stages; (2) identify statistically significant spectral intervals and spatial patterns of scattering reflectance between healthy and diseased onion bulbs; (3) determine the depth of light propagation in healthy and infected bulbs in the VIS and NIR spectral range; and (4) validate the simulation results of healthy bulbs using experimental data.

2. Materials and methods

2.1. Input optical properties for MCML simulations

Optical properties $\{\mu_a, \mu_s, g\}$ of onion tissues were previously computed from the experimentally measured optical responses $\{R, T, T_c\}$ by Wang and Li (2014) and a summary of the median optical properties at 800 nm were provided (Table 1). There were six types of onion tissues: healthy onion dry skin (HLDry), healthy onion flesh (HLFlesh), Neck Rot-infected dry skin (NRDry), Neck Rot-infected flesh (NRFlesh), Sour Skin-infected dry skin (SSDry), and Sour Skin-infected flesh (SSFlesh). Here μ_a is absorption coefficient in units of cm^{-1}, μ_s, is scattering coefficient in units of cm^{-1}, g is dimensionless scattering anisotropy factor, R is dimensionless tissue's reflectance, T is dimensionless tissue's transmittance, and T_c is dimensionless tissue's collimated transmittance. The measured optical properties cover the spectral range from 530 to 1650 nm with a step size of 2 nm.

Data pre-screening was applied to the original dataset to remove unreliable replicates which were affected by noise in experimental setup and by convergence issues in the Inverse Adding–Doubling (IAD) program (Prahl et al., 1993) that was used for conversion of the optical responses $\{R, T, T_c\}$ to optical

Table 1
Optical properties (median) of healthy, Neck Rot (NR)-infected, and Sour Skin (SS)-infected tissues at 800 nm (optical properties for other wavelengths can be found in Wang and Li (2014)).

	Dry skin			Flesh		
	μ_a (cm^{-1})	μ_s (cm^{-1})	g	μ_a (cm^{-1})	μ_s (cm^{-1})	g
Healthy	1.528	291.775	0.4111	0.171	20.554	0.4878
NR infection	2.301	344.295	0.3887	0.644	17.703	0.6138
SS infection	2.023	344.935	0.4975	0.339	11.103	0.7583