Lasers in Medical Science (2023) 38:96
https://doi.org/10.1007/s10103-023-03758-6

ORIGINAL ARTICLE

Modeling optical fluence and diffuse reflectance distribution in normal and cancerous breast tissues exposed to planar and Gaussian NIR beam shapes using Monte Carlo simulation

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Received: 16 August 2022 / Accepted: 28 March 2023

Abstract
Precise knowledge about light propagation in biological tissues is necessary for accurate diagnostics and effective therapies utilizing optical technologies. In the current paper, the Monte Carlo simulation is applied to study light dispersion in normal and cancerous breast after irradiating to different laser beam shapes. Two distinct laser wavelengths (800–1100 nm) with planar and Gaussian shapes were employed. The spatially resolved steady-state diffuse reflectance of normal tissue and tumor was investigated using Monte Carlo simulation method via MCML and MCXLAB computations. The diffusion equation was solved to simulate the fluence rate at the tissue surface based on the optical parameter values (i.e., scattering and absorption coefficients). The results confirm differences in diffuse reflectance and optical fluence distribution between the normal and tumor tissues at each wavelength. Tissue optical parameters and the utilized laser beam shape control the distribution of the fluence rate within tissues. Therefore, offering visual representations of these distributions can provide a secure visual route for biological diagnostics.

Keywords Diffuse reflectance · Fluence rate · NIR laser · Tissue optical parameters · Beam shaping

Introduction

The second-leading cause of cancer-related mortality is breast cancer. This type of cancer can affect both genders; however, it is mostly diagnosed in women. By contrasting breast cancer fatalities among women with ductal carcinoma in situ (DCIS) diagnoses with anticipated breast cancer deaths among women in the general population who did not have cancer, ratios of standardized mortality were calculated [4, 12]. Because glandular tissue experiences more lesions than any other layer [12], malignant diseases are modeled in that layer. Therefore, early detection of breast cancer is critical for the disease prevention. Nowadays, MRI, X-ray, ultrasound, CT, and frozen pathological examination are the common breast cancer screening techniques [10, 12]. While the present approaches could be improved, a non-destructive, cost-free, and more precise approach is also required.

For appropriate use of light (especially lasers) in medical diagnostic and therapeutic purposes, it is essential to comprehend how the laser beam interacts with the tissue. The optical characteristics of the tissue affect how light travels through biological materials. The chance of light absorption inside biological tissue is known as the absorption coefficient (μ_a), and it provides details on the concentration of light-absorbing molecules, known as tissue chromophores. On the other hand, the concentration, size, and form of the scattering molecules affect the scattering coefficient (μ_s), which is the chance of light scattering inside the tissue. In addition, the anisotropy factor (g) measures how much the direction changes as a result of scattering from light-absorbing and light-scattering molecules. It is also the mean cosine of the deflection angle caused by photon scattering. Fundamentally, these parameters are wavelength-dependent [12].

Since the scattering coefficient is known to be substantially larger than the absorption coefficient in biological material, there are only few clinical applications for optical technologies. As a result, scattering and absorption

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Published online: 01 April 2023

characteristics are crucial markers for tissue health and support diagnostic techniques [3, 16]. Additionally, the analytical investigation of the light scattering and absorption inside the tissue is a difficult process due to the complex structure of biological tissues Therefore, several computational techniques have been introduced in order to analyze the light propagation inside the tissue. Radiative transport theory [13, 18], the Kubelka–Munk model [9], the multi-flux model [22], the adding-doubling method [14], and diffusion approximation [15] are among the most widely used mathematical and numerical techniques implemented in previous studies. Additionally, Monte Carlo (MC) simulation method has been broadly and successfully applied to simulate photon transport and describe light distribution in tissues. It is considered a gold standard for analyzing how light propagate within biological tissue.

Breast tumor at various depths was identified using MC simulation utilizing near-infrared fluorescence [14]. The use of near-infrared (NIR) wavelengths in the detection of various diseases has been introduced providing provision of low-risk, low-cost, real-time, and non-destructive approach. NIR-I (i.e., 750–1000 nm) and NIR-II (i.e., 1000–1700 nm) photons, also known as "biological transparent windows," have the greatest penetration depth as tissues in these wavelength ranges have lower absorption and scattering coefficients [3, 11, 16] and exhibit less autofluorescence, making them suitable for use in bio-photonic imaging. Therefore, smaller, deeper-seated tumors can be easily detected using NIR fluorescence[20].

The detected transmitted and/or reflected signal becomes diffuse when NIR light is used to illuminate the tissue. Diffuse reflectance spectroscopy (DRS) is an optical technology that reflects the composition and morphology of tissue by measuring the interaction between light and tissue. A DRS measurements provide information on the optical characteristics of tissue, which can be applied to discriminate different tissue types [5]. However, laser propagation in tissue influenced by the laser beam characteristics, such as power, spot size, time of exposure, pulse repetition rates (in the case of pulsed lasers), beam width, wavelength, and beam shapes [2]. A flat top laser beam is a beam whose intensity profile is uniform with a certain beam shape and a sharp drop-off at the edges [17]. This type of beam profiles has almost no dependence between energy and spot size above the threshold [7]. This makes a flat top beam profile highly desirable in many laser applications. On the other hand, the Gaussian beam profile is the most common laser beams shape, where the width of the Gaussian spot is directly proportional to the energy [19].

This research sets out to determine how various NIR laser wavelengths and beam shapes affected the dispersion of light in normal and malignant breast tissues. In order to distinguish between the light distribution inside of normal and tumorous human breast tissues, the distributions of fluence rate and spatially resolved steady-state diffuse reflectance of the light with various NIR wavelengths starting from 800 to 1100 nm in different beam shapes were used. The simulation's output uses MCML to provide spatially resolved steady-state diffuse reflectance profiles of the tissues under examination. The optical parameters were then added to the diffusion equation in order to generate images of the fluence rate distribution using MCXLAB.

Methods

The precise goals of this work were to simulate the dispersion of light in breast tissue using various combinations of optical characteristics and laser beam shapes, in addition to compare the diffuse reflectance and the fluence rate distribution generated by different NIR laser wavelengths were obtained in normal and tumorous breast tissue. MC simulation can model the propagation of light through three-dimensional (3D) tissue as a process of random walk with a good approximation to reality. The MC model has been utilized to address a number of issues in the physics of light propagation in biological tissue. It is a stochastic model [21] of the transport of photons in a medium in which there are established rules for the interactions of light inside the medium. The wavelength-dependent optical tissue characteristics, including the coefficients of absorption μ_a and scattering μ_s, control how light interacts with tissue.

The distribution of light within the tissue is simulated by solving the radiative transfer equation. The GPU-based MC eXtreme model developed by [6] served as the basis for the light transport model used in this work and also the MC code applied to multi-layered tissues (MCML) by [21].

Diffusion equation

The diffusion equation is a partial differential equation that approximates the radiative transport equation by assuming that the radiation is almost isotropic and is much simpler to solve than the equation of radiative transport, which can be stated as [8]:

$$\frac{\partial \phi\left(\vec{r},t\right)}{c\partial t}+\mu_a\phi\left(\vec{r},t\right)-\nabla.\left[D\nabla\phi\left(\vec{r},t\right)\right]=S\left(\vec{r},t\right) \quad (1)$$

where $D=\left[3\left(\mu_a+\acute{\mu}_s\right)\right]^{-1}$ is the coefficient of diffusion, $\phi\left(\vec{r},t\right)$ is the rate of fluence in (W/cm^2), $S\left(\vec{r},t\right)$ is the source of isotopic in (W/cm^3 sr), and $\acute{\mu}_s$ is the decreased coefficient of scattering, which is equal to $\left((1-g)\mu_s\right)$, where g represents