UCT JOURNAL OF SOCIAL SCIENCE AND HUMANITIES RESEARCH 2014(03)

Available online at http://journals.researchub.org

Numerical Study of Optical Properties and the Effect of Anisotropy on a Tissue by Using Monte Carlo Method

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ARTICLE INFO

Article history:
Received 22 Jun 2014
Received in revised form 23 Jul 2014
Accepted 06 Aug 2014

Keywords:
Numerical Study
Anisotropy
Monte Carlo
Method

ABSTRACT

Objective: During the last few decades, a variety of medical scanning devices has been made and each, considering its unique features, has many applications. **Methodology:** In this paper efforts have been made to use Monte Carlo method to simulate the trajectory of the photons in biological tissue. New features were added to the Monte Carlo simulation. In this paper, of the most prominent features of simulation, changing the angle of incident beam to the tissue, selecting multilayer tissues, and choose the type of tissue could be named. In this study the results compared with others and the also the effect of anisotropy on the optical properties of the tissue were examined. **Results:** The results obtained with this code, even using a relatively small number of photons, compare favorably with those obtained elsewhere. The code can be changed so that the number of grid points is read as data input. It is worth emphasizing though that, with the option of running the Monte Carlo simulation directly from the code. **Conclusion:** the results obtained with the Monte Carlo simulation for different entry angles. No similar calculations have been found in the literature for a comparison to be possible. Our results seem to indicate that the diffuse reflectance and absorbance increases with decreasing angle while the transmittance decreases.

1. Introduction

The optical properties of a tissue affect both diagnostic and therapeutic applications of light. The ability of light to penetrate a tissue, interrogate the tissue components, and then escape the tissue for detection is key to diagnostic applications. The ability of light to penetrate a tissue and deposit energy via the optical absorption properties of the tissue is key to therapeutic applications (Mommas, 2004 and Côté & Vitkin, 2005). Hence, specifying the optical properties of a tissue is the first step toward properly designing devices, interpreting diagnostic measurements or planning therapeutic protocols. The second step is to use the optical properties in a light transport model to predict the light distribution and energy deposition. In this paper we will study and focus on the light transport model with Monte Carlo simulation which is based on random variables. There are reviews that tabulate the optical properties of various tissues (Jacques, 2013). Modeling photon propagation with the Monte-Carlo methods is a flexible yet rigorous approach to simulate photon transport. In the method, local rules of photon transport are expressed as probability distributions which describe the step size of photon movement between sites of photon-tissue interaction and the angles of deflection in a photon's trajectory when a scattering event occurs. This is equivalent to modeling photon transport analytically by the radiative transfer equation (RTE), which describes the motion of photons using a differential equation (Reckwitz, 2009). However, closed-form solutions of the RTE are often not possible; for some geometries, the diffusion approximation can be used to simplify the RTE, although this, in turn, introduces many inaccuracies, especially near sources and boundaries. In contrast, Monte Carlo simulations can be made arbitrarily accurate by increasing the number of photons traced. The Monte Carlo method is necessarily statistical and therefore requires significant computation time to achieve precision. In addition Monte Carlo simulations can keep track of multiple physical quantities simultaneously, with any desired spatial and temporal resolution. This flexibility makes Monte Carlo modeling a powerful tool. Thus, while computationally inefficient, Monte Carlo methods are often considered the standard for simulated measurements of photon transport for many biomedical applications (Jacques, 2013).

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DOI: https://doi.org/10.24200/jsshr.vol2iss03pp62-69

1.1. Biology Monte Carlo methods

Monte Carlo methods are a broad class of computational algorithms that rely on repeated random variables to obtain numerical results. The Monte Carlo methods are very important in computational physics, and other related applied fields especially in computational biology. Biological systems such as tissues are being studied by means of computer simulations. The systems can be studied in computer simulations which allow us to monitor the local environment of a particular tissue to see if some interaction is happening for instance. Biology Monte Carlo methods (BioMOCA) have been developed at the University of Illinois at Urbana-Champaign to simulate ion transport in an electrolyte environment through ion channels or nano-pores embedded in membranes (Wilson & Adam, 1983). This method is now widely applied to simulate photon-tissue interaction. The Monte Carlo simulation described in this paper deals with the transport of an infinitely narrow photon beam incident on a tissue at any angels. The layers of the tissue are described by the following parameters: the thickness, the refractive index, the absorption coefficient and the scattering coefficient (Rafieian, 2010). Table 1. Shows the coefficient for some tissues. When a beam of photons encounters a given media such as biological tissue, each particle undergoes a succession of interactions with the atoms of media and at each collision two fates are possible: (i) either the photon is captured and disappearing from the beam, or (ii) the photon is scattered thus moving into a different direction with the same energy if it undergoes an elastic collision or possibly with different energy if the collision is inelastic. Since one cannot follow a photon in a microscopic dimension and predict what is going to happen to it, we should study the event statistically and show the results as a probability of a given outcome to occur. This means that photon-tissue interaction obeys statistical laws. The probability that a photon captured or scattered is given by cross-section. If we show the cross-section for capture and cross section for scattering with σc and σs then the total cross-section, and the captured and scattered probabilities are then determined as $\sigma t=\sigma c+\sigma s$, $pc=\sigma c/\sigma t$ and $ps=\sigma s/\sigma t$ respectively. One may describe the capture and scattering in terms of the coefficient of absorption (μa) and scattering (μs). Here we consider a biological tissue, on which the beam of photons is incident and it has a finite path. As shown in Fig. 1, a photon may be transmitted, or may be captured/absorption, or may be reflected through the same boundary it entered as a result of one or more bounce-back collisions suffered inside the material.

Table 1. Examples of optical tissues properties

Tissue	λ [nm]	μ_s [cm^{-1}]	μ_a [cm^{-1}]	anisotropyfactor
aorto	633	31	3.1	0.90
bladder	633	29.3	1.4	0.91
$brain_{[whitematter]}$	633	51	1.58	0.96
$brain_{[graymatter]}$	633	60.2	2.63	0.88
liver	630	414	3.2	0.95
lung	635	324	8.1	0.75
skin	633	187	2.7	0.81

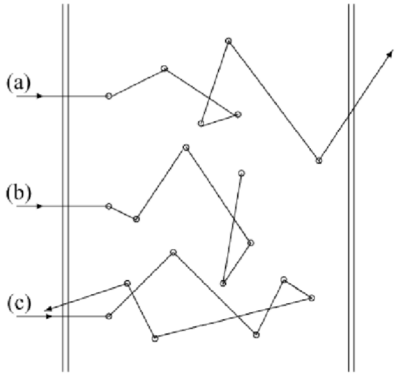

Figure 1. Three scenarios for a particle/photon

Three scenarios for a particle/photon incident on a material layer of finite depth: (a) the particle/photon traverses the layer and comes out through the opposite boundary; (b) the particle/photon is absorbed inside the layer; (c) the particle/photon is reflected back leaving the tissue through the boundary it went in. There are many Monte Carlo codes available such as Monte Carlo-Diffusion hybrid method Jacques (2013), Monte Carlo code for photon migration though 3D media with spatially varying optical properties (Wang & Jacques, 1994). Each code is concentrated on particular features. In this paper the simpler Monte Carlo standard C code of Wang et al, (1995). Boas et al. (2002), is considered. Our codes are written with Maple programming language.

The paper is structured as follows. In section III we examine the structure of simulation and describe random variables for the simulation. The last section is dedicated to show the results of the simulation and their comparison with others.

2. Materials and Methods

The Monte Carlo methods are based on random variables from probability distribution. Variable x is a random variable if it can take an arbitrary value in a given interval [a,b], with a specified probability. The probability density function p(x) satisfy

$$\int_a^b p(x)dx = 1 \quad (1)$$

On the other hand, random values are generated by computer are distributed over interval [0,1]. It can be shown that the values of a random in a given interval [a,b] can be obtained from interval [0,1]. If κ is a given value of the random variable uniformly distributed in over the interval [0,1] then the value of the non-uniform variable x with probability density function p(x) can be found by solving integral

$$\int_0^r p(x)dx = \kappa \quad (2)$$

Photon has a Brownian motion in the tissue. So one should assign two variables to the particle. The associated random variables are free path length and the direction in which the photon moves after being scattered. The latter is defined by the cosine of the directional angles. The step size of the photon packet is calculated based on a sampling of the probability distribution for photon's free path s belongs to [0,∞) Its probability density function is given by

$$p(s)ds = \mu_t e^{-\mu_t s} ds \quad (3)$$

Where μ_t is he total (absorption plus scattering) interaction coefficient. Using eq. (2) and (3) one can obtain step size S for the free path length variable.

$$s = -\frac{\ln(1-\kappa)}{\mu_t} = -\frac{\ln(r)}{\mu_t} \quad (4)$$

Where κ and r are random uniform variable over the interval [0,1]. One has to define the deflection angle θ ($0 \le \theta \le \pi$) and azimuthal angle φ ($0 \le \varphi \le 2\pi$) for direction followed by

$$p(\cos\theta) = \frac{1-g^2}{2(1+g^2-2g\cos\theta)^{\frac{3}{2}}} \quad (5)$$

Where g($-1 \le g \le 1$) is the average value of cosθ and characterize the anisotropy of tissue.

$$\cos\theta = \begin{cases} \frac{1}{2g}\left(1+g^2-\left(\frac{1-g^2}{1-g-2gr}\right)^2\right) & g \neq 0 \\ 2r-1 & g = 0 \end{cases} \quad (6)$$

As far as the azimuthal angle is concerned, its sampling is $\varphi = 2\pi r$ since this is uniformly distributed over the interval [0, 2π]

2.1. Programming

The assumptions and programming steps of this code follow closely those of Wang et al, (1995).'s C program (Boas et al., 2002). Photons are treated as classical particles, polarization and wave phenomena are neglected, and a packet of photons is used instead of a single photon. The packet is characterized by a given weight function w, whose initial value is set equal to 1 (w_0=1). All photons travel together and are scattered together like a single photon. However, when absorption occurs at some point, the packet does not disappear completely but instead its weight function decreases. Each photon packet is able to pass one or more tissue layers surrounded by air. The macroscopic optical properties of a tissue also identified with any microscopic volume of that tissue. Grid systems are used to consider photon absorption and scattering events at different locations (Lemoigne & Caner, 2010, Mohammadi & Majidifar, 2010).

Wang et al, (1995).'s code Boas et al. (2002), considers only normal incident and infinitely wide layer. In contrast, our code allows to choose the incident angle for first layer as well as the geometry of the tissue layers. It is assumed infinitely wide, cylindrical, and prismatic geometries. Each packet start its interaction from (x,y,z)=(0,0,0). Fig 2. shows the direction of the xyz axes versus the orientation of the layers. The angles that the direction of incidence make with the x and y direction is

$$\cos\theta_x = \cos\theta_y = \frac{1}{2}\sqrt{1-cos^2\theta_z} \quad (7)$$

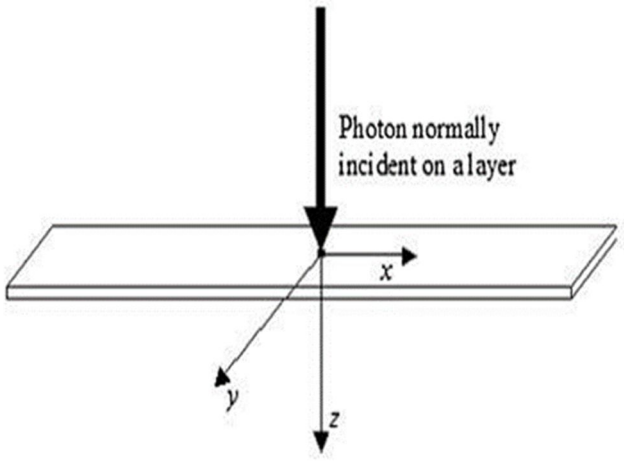

Figure 2. The direction of the xyz axes versus the orientation of the layers.

At the initial launch of every photon, partial reflection occurs contributing to the specular reflectance. However, the weight of the photon that enters the first layer is affected by this event. At every point of the photon's path in a given tissue i, the step size is compared to the distance between that point and

the boundary with the tissue j towards which it is heading. If the step size is smaller than this distance, then part of the weight function is absorbed and the remaining weight function is carried by the scattered packet. At such interaction point, the absorbance is then increased by

$$\Delta w = w\frac{\mu_a}{\mu_t} \quad (8)$$

If the step size is larger than the distance between the path's current point and the boundary towards which the packet is heading, further checking is necessary to determine whether the packet is transmitted or reflected. Let's denote by α_i and α_j the angles that the direction of the photon makes, in media i and j and respectively. These angles satisfy Snell's law ($n_i \sin \alpha_{i=} n_j \sin \alpha_j$). If is greater than the critical angle for this interface, total internal reflection occurs but, if it is smaller, the possibility of internal reflection is not dismissed right away. By introducing internal reflection parameter one can compare random variable for step size.

If $r \leq R(\alpha_i)$ internal reflection occurs, else the packet is transmitted onto the tissue layer j . Then both the direction of propagation and the step size are updated. When the j th layer labels the ambient air at the top and the bottom, the diffuse reflectance and the transmittance is updated respectively. In either case, it is assumed that the quantity in question increases by $w(1-R(\alpha_i))$ instead of w . This assumption is expected to w lower the variance of the results (Boas et al., 2002). There is a threshold value w_{th} when the weight function decreases. According to Wang et al, (1995). Boas et al. (2002), the threshold value is set equal to 0.0001. The fate of the current photon packet is, at that point, decided by comparing the aforementioned random number r with the ratio 1/m where m is an arbitrary integer which is set equal to 10 (Boas et al., 2002). If $r \leq 1/m$ the weight is increased tov mw_{th} and the photon packet continues on; else the current photon is dead and a new photon is launched. Finally when the simulation has used up all the photons, the accumulated values of the specular/diffuse reflectance, transmittance and absorbance are normalized by dividing the total amounts by the number of photons.

3. Results and Discussion

The following grid values are assumed in all runs of program.

i. For the exit angle, the total number of grid points and the grid resolution are Na=30, da= $\pi/2$Na respectively.

ii. For the radial direction, the total number of grid points and the grid resolution are Nr=200, dr= 0.005 respectively.

iii. For the depth, the total number of grid points and the the grid resolution are Nz=20, dz= total d/Nz respectively. Where totald is the summation over all thicknesses of the tissue layers.

Table 2. shows the results of several runs which is performed with the same tissue parameters but different number of photons. According to Fig. 4 as expected, the computation time increases rapidly with the number of photons used in the simulation.

Table 2. Comparison of results obtained in several runs of the code with different number of photons

Specular reflectanc	Diffuse reflectance	Absorbtion	Transmission	number of photons	Run Time
0.02006	0.2130	0.2335	0.5334	500	69s
0.02006	0.1896	0.2416	0.5487	1000	142s
0.02006	0.1819	0.2554	0.5426	2000	~285s
0.02006	0.1877	0.2538	0.5385	5000	~750s
0.02006	0.1951	0.2473	0.5375	10000	~1720s

All runs were for one 1.0 cm thick tissue layer with the following properties: index of refraction n=1.33, absorption coefficient μa=0.1 cm-1, scattering coefficient μs=10 cm-1 and anisotropy g=0.93. The incidence of the photons is normal (Boas et al., 2002).

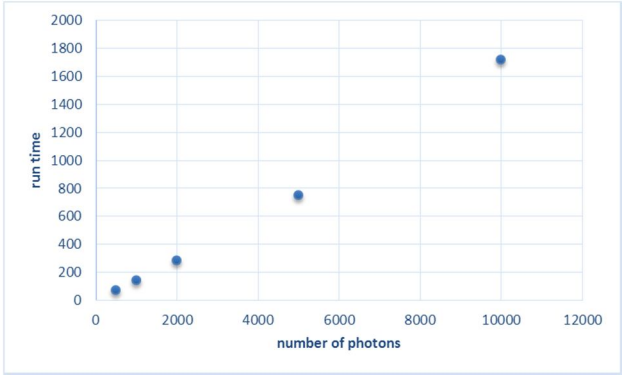

Figure 3. Several runs of the code with different number of photons as shown in table 1.

Fig. 4-5 shows optical properties of tissue vs. depth, angles and radius with 10000 photons respectively. As shown in Fig. 7, absorption and diffusion reflectance decreases by increasing angle. But the transmittance increses.

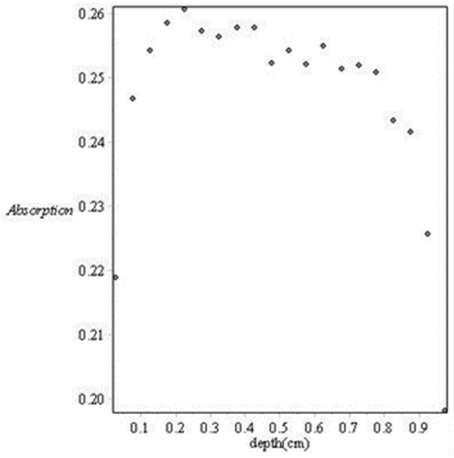

Figure 4. Plot of absorption vs. depth for a biological tissue with

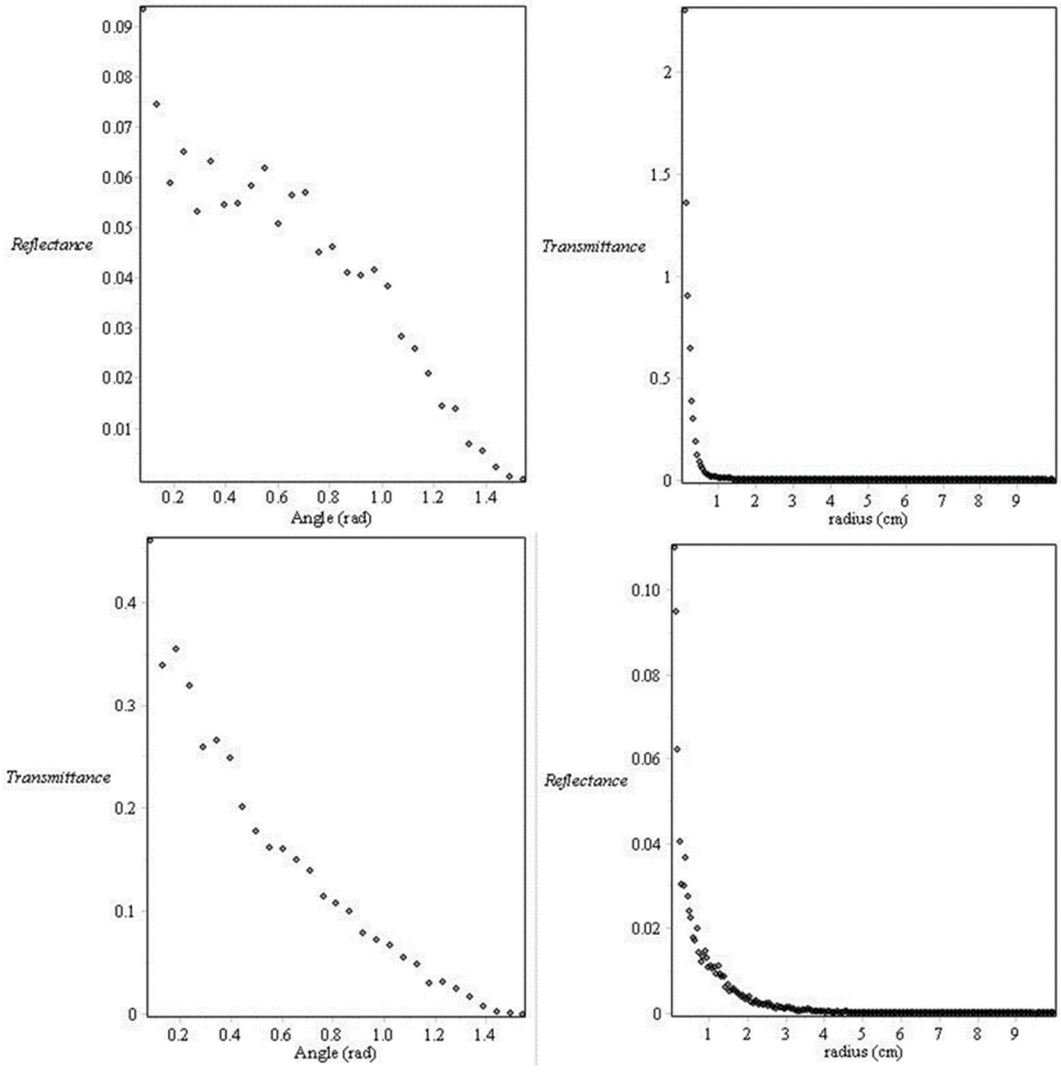

Figure 5. Radially and angularly resolved. Transmittance vs. radius and angle respectively with 10000 photons.

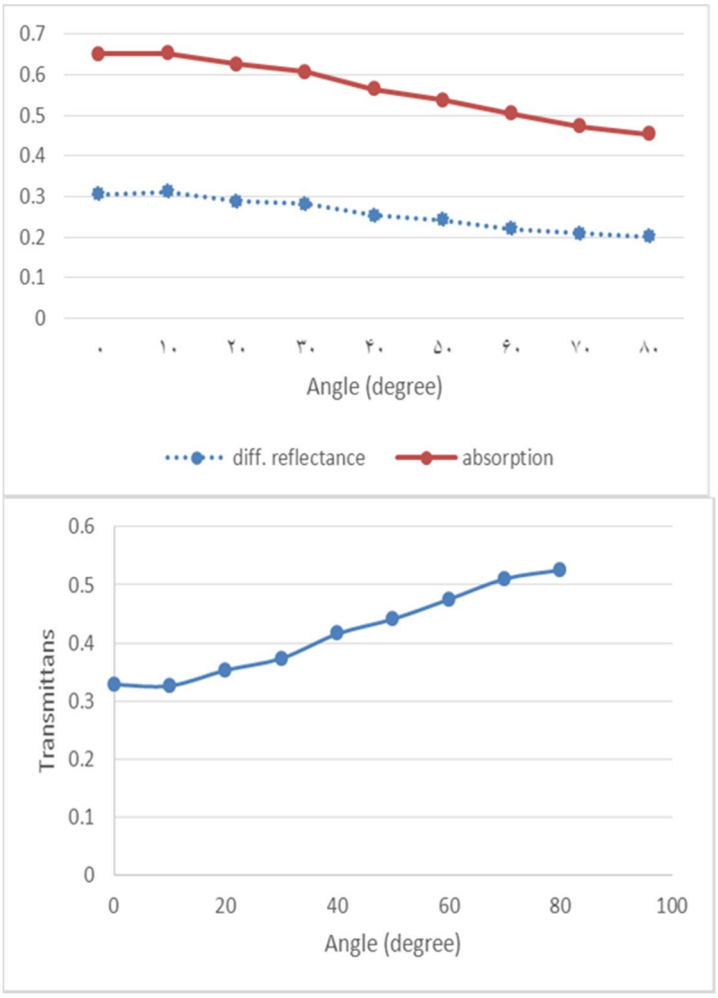

Figure 6. Absorption, diffusion reflectance and transmittance vs angels of incident beam.

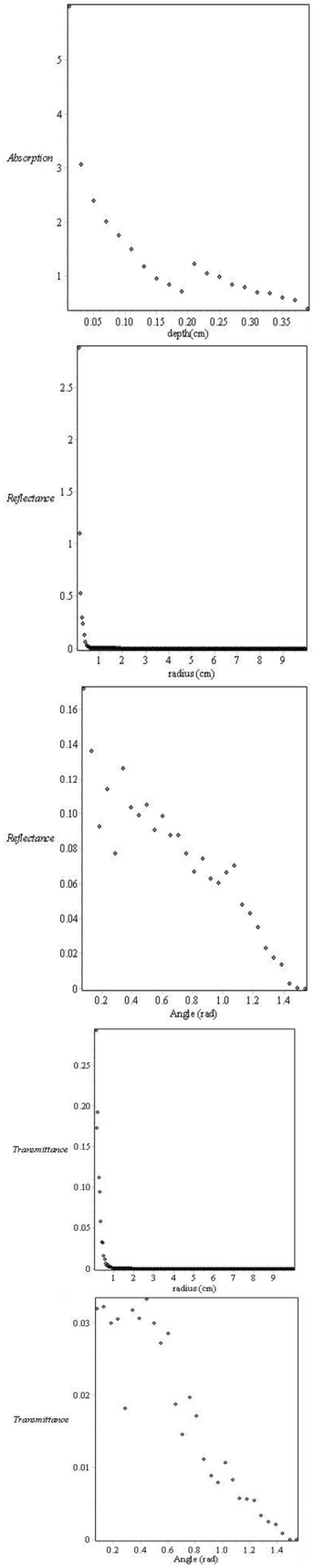

Figure 7. The Monte Carlo simulation for a three-layer tissue.

Fig 8. shows the Monte Carlo simulations for an infinite layer with various optical properties, and fitted the run times as a function of the ratio between scattering coefficient and absorption coefficient (μs/μa) and anisotropy g.

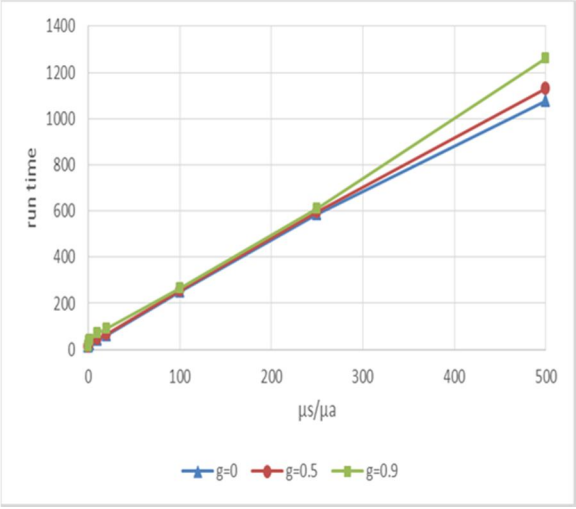

Figure 8. The run time vs. ratio between scattering and the absorption coefficient for different anisotropy factor of tissue.

4. Conclusion

In conclusion, we present a Maple code particularly adept to simple Monte Carlo simulations of photon transport in tissue layers. The results obtained with this code, even using a relatively small number of photons, compare favorably with those obtained elsewhere. The code can be changed so that the number of grid points is read as data input. It is worth emphasizing though that, with the option of running the Monte Carlo simulation directly from the code. We also display the results obtained with the Monte Carlo simulation for different entry angles. No similar calculations have been found in the literature for a comparison to be possible. Our results seem to indicate that the diffuse reflectance and absorbance increases with decreasing angle while the transmittance decreases.

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How to Cite this Article:

Ghahramani A., Eskandari S., Numerical Study of Optical Properties and The Effect of Anisotropy on A Tissue By Using Monte Carlo Method, Uct Journal of Social Sciences and Humanities Research 03 (2014) 62–69.