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Monte Carlo model for reflectance Pulse Oximetry using pulsatile monolayer perfused skin tissue

S Chatterjee*, P A Kyriacou

Research Centre for Biomedical Engineering (RCBE), City, University of London, UK, EC1V0HB

*Email: subhasri.chatterjee.1@city.ac.uk

Abstract. Pulse Oximetry (PO) is a non-invasive method for estimating arterial oxygen saturation from Photoplethysmography signals recorded from peripheral tissue sites. Despite a very wide range of clinical applications, the fundamental working principles of PO is still not very well understood. In this work, a Monte Carlo model is executed for a monolayer volume of human skin dermis in a reflectance detection modality to investigate the basic nature of light-tissue interaction in the tissue. Differences in systolic and diastolic blood volume explained the pulsatility. The distribution of light-tissue interaction was illustrated, systolic and diastolic reflectance at red and infrared light were simulated and the ‘calibration curve’ was produced.

1. Introduction

Oxygen saturation is the measure of the fraction of the oxygenated hemoglobin to the total hemoglobin present in the blood. Oxygen saturation measured from the arterial blood is a critical parameter for patient monitoring. A value of arterial oxygen saturation ($\text{SaO}_2$) as low as 60% is known as hypoxemia which is a serious condition denoting that patient is not acquiring adequate oxygen, which if left untreated leads to end of patient life. Therefore, continuous monitoring of arterial oxygen saturation is of utmost importance [1].

Pulse Oximeter (PO), a non-invasive tool for continuous arterial blood oxygen saturation measurements, is a standard of care in clinical emergency, neonatal and anesthesiology units. The working principle of PO relies on a volumetric measurement technique known as Photoplethysmography (PPG). In this non-invasive procedure, light is emitted from a source to the tissue surface and the reflected/ transmitted light is detected. In this method, the ‘AC’ pulsatile PPG signal associated with cardiac contraction is assumed to be attributable solely to the arterial blood component. On the other hand, the slowly varying ‘DC’ component of the PPG signal is considered to be produced due to the absorption in non-pulsatile tissue compartments. The amplitudes of the red and infrared AC PPG signals are sensitive to changes in arterial oxygen saturation because of differences in the light absorption of oxygenated and deoxygenated hemoglobin at these two wavelengths. From the ratios of these amplitudes, and the corresponding dc photoplethysmographic components, arterial blood oxygen saturation from the peripheral tissue ($\text{SpO}_2$) is estimated [2].

Although the clinical reliability of PO measurements is globally accepted, the basic understanding of the fundamental aspects of this technique is not yet clearly understood. In the present age of wearable sensor technology, in order to optimize or miniaturize the design of a sensor, it is very important to have an in-depth knowledge on the fundamental working principle of the technique,
which is missing in this case. There is no available modelling study which discusses all the crucial parameters such as the intensity and penetration depth in PO. These parameters are important not only for a better understanding but also, in order to optimize the sensor design and modify it to a calibration-free technology.

A single layer pulsatile Monte Carlo model was used to investigate the dependence the detected light intensity on blood volume and blood oxygen saturation in a tissue with the optical properties of skin (dermis) containing blood. The Monte Carlo method is a well-known technique for solving problems related to light-tissue interaction that are too complex to solve analytically [4-6]. Using this method, a reflectance pulse oximetry probe was simulated, emitting two commonly used optical wavelengths for pulse-oximetry, 660 and 940 nm, onto skin dermis tissue. The model was explored to demonstrate the distribution of the interaction between the optical signal and the tissue, and evaluate the parameters such reflectance to produce the ‘calibration curve’ of Pulse Oximetry.

Traditionally, the pulse oximeters are empirically calibrated by creating a dataset on the experiment on a large number of healthy volunteers [10]. The normal oxygen saturation of a healthy person is above 95%. For the empirical calibration, the low level of oxygen saturation is artificially created in the volunteers. This method is restricted ethically to get any data below 70% oxygen saturation, thus the calibration curves for commercial pulse oximeters are extrapolated for very low oxygen saturation values. This approximation does not really impose any limitation on the clinical measurements, as a patient with an oxygen saturation value as low as 70% is an extremely critical condition and other methods are then applied to improve patient’s condition. Nevertheless, a theoretical or modelling based concept to generate the calibration curve of such an important medical device is useful for the future possibility of a calibration-free Pulse Oximeter.

2. Methodology
In a typical Monte Carlo optical model, virtual photon packets are simulated as they pass through a volume of tissue which is, in general, a highly scattering and partly absorbing medium with known optical properties. These properties are defined as the scattering coefficient $\mu_s$, absorption coefficient $\mu_a$ and scattering anisotropy $g$, each being dependent on the photon wavelength $\lambda$. The steps of the Monte Carlo methodology have been explicitly described in our earlier publication [7]. Light-tissue interaction was simulated in a three-dimensional volume of tissue which was represented by a slab-geometry of an infinite width. In the reflectance setting, the source-and the detector was considered to be placed on the tissue surface. Entire system was presented in a 3D Cartesian co-ordinate system.

The ‘pulse’ in this model was achieved by increasing the diastolic ($\text{diast}$) arterial blood volume, i.e. 5% in systole ($\text{syst}$) by 2%. The venous blood volume, i.e. 5% was assumed to be unaffected by the pulse, with a venous oxygen saturation lesser by 10% than $\text{SaO}_2$. It was considered that the slab thickness was 1 cm and source-detector separation was 6 mm. Gaussian beam of 1 mm radius was made incident to the model. The detector diameter was 1 mm. The modulation of light attenuation in the systolic and diastolic states is the main origin of the PPG signal. The main optical parameter responsible for attenuating light propagation through it is the absorption coefficient. The effective absorption coefficient of the dermal tissue takes into account the contribution of the main absorbers, i.e. oxyhemoglobin and deoxyhemoglobin.

The baseline absorption coefficient $\mu_{a_{\text{baseline}}}$ i.e., the absorption coefficient of the skin tissue sublayers due to the intrinsic absorption property only in absence of any other chromophore at an operating wavelength $\lambda$ is given by the equation below [7,8]:

$$\mu_{a_{\text{baseline}}} (\lambda) = 7.84 \times 10^7 \times \lambda^{-3.255}. \tag{1}$$

The absorption coefficient of skin is written as [11]:
\[
\mu_a(\lambda) = V_A \mu_a A(\lambda) + V_V \mu_a V(\lambda) + [1 - (V_A + V_V)] \mu_a \text{baseline}(\lambda)
\]  

(2)

where \(V_A\) and \(V_V\) stand for the arterial and venous blood volume-fraction respectively \((V_V = V_A / 2)\), and \(\mu_a, \mu_A, \mu_V\) are the absorption coefficients of the arterial blood, venous blood and water. The absorption coefficients of arterial and venous blood basically attribute to the absorption properties of oxy and deoxyhemoglobin, as stated in the following equations [7]:

\[
\mu_a A(\lambda) = S_a O_2 \mu_a A HbO_2 (\lambda) + (1 - S_a O_2) \mu_a A HHb (\lambda)
\]  

(3)

\[
\mu_a V(\lambda) = S_v O_2 \mu_a V HbO_2 (\lambda) + (1 - S_v O_2) \mu_a V HHb (\lambda)
\]  

(4)

where and \(\mu_{ox}\) are the absorption coefficients of oxy and deoxyhemoglobin, \(S_a O_2\) and \(S_v O_2\) are the arterial and venous oxygen saturation respectively \((S_v O_2 = S_a O_2 - 10\%)\).

The hematocrit of blood was considered to be 45%. The absorption coefficients of the blood constituents (HHb and HbO) were adapted from literature [9]. The code was written in MATLAB® platform.

In the Monte Carlo algorithm, the light beam is considered as a packet of photons, which is introduced with an initial ‘weight’, \(w=I\). This weight is not physically same with the light intensity; however, it carries an equivalent meaning to the energy or the intensity of light beam. As the photon-packet moves throughout the tissue structure by a step size calculated from the random sampling of the probability of photon free pathlength [7, 11], it encounters absorption events. In each absorption, a certain amount of the photon weight or energy is absorbed, which can be calculated as \(\Delta w = \mu_a \Delta x \cdot w\) and the remaining weight of the photon packet is subjected to the ‘scattering’ event and orients to a new direction. The photon packet continues to propagate through tissue until it exits the medium or lost within tissue medium. Due to numbers of absorption, if the remaining photon weight is too small, the information carried by that photon is negligible, thus discarded. In the reflectance geometry, the source and detector were assumed to be placed on the same side of the tissue. Photons emitted from the top surface were checked if they fell within the ‘detection criteria’, i.e., if their point of emission lied within the area of the detector. If the criteria had met, the photon was ‘detected’ and the ‘reflectance’ \(I\) was measured which was basically the remaining weight of the photon packet. The photons emitting through the bottom surface of the tissue or through the top surface not satisfying detection criteria, were discarded. The simulations were run to detect 10\(^7\) photon packets in the geometrical setting, each for systole and diastole at both red and infrared wavelengths.

The reflectance in the systolic and diastolic states \(I_{sys}\) and \(I_{dia}\) respectively) at red (\(r\) and infrared (\(i\) wavelengths were executed for a range of arterial oxygen saturation \((S_a O_2 = 10-100\%)\). These measurements lead to the quantification of the ‘ratio of ratios’ \(R\), as a function of \(S_a O_2\), following the equation written below [10]:

\[
R(S_a O_2) = \frac{I_{sys}(S_a O_2)}{I_{dia}(S_a O_2)} r \quad \frac{I_{sys}(S_a O_2)}{I_{dia}(S_a O_2)} i
\]  

(5)
3. Results and discussion

Figure 1. Densityplots of the Monte Carlo simulated distribution of the interaction events $N$ (i.e., scattering-absorption) through the dermal skin tissue are presented for 660 nm and 940 nm in (a) and (b) respectively. The directions of entry and transmission of the photon packets are indicated by red arrows. The colourbar represents the distribution of the colour in the desityplot-images between the minimum and maximum values of the interaction events. For comparison, both images have been shown in the same scale.

The interaction between light and tissue in a typical reflectance Pulse Oximetry geometrical setting is illustrated in figure 1. The densityplots of the distribution of the interaction events (scattering and absorption) within the dermal skin tissue for 660 nm and 940 nm wavelengths for source-detector separation 6 mm are presented in figure 1(a) and 1(b) respectively. The photons are incident on the tissue surface ($z=0$) at the point $(0,0,0)$ to form a Gaussian beam. The photons emerging through the area of the detector having a centre at $(6,0,0)$ are detected. In the two wavelengths, the distribution of the photon scatter is different. The infrared photons penetrate deeper compared to the red photons, however, the red photon scatter distribution is more compact than infrared. The optical path of photon through tissue is mainly governed by the scattering coefficient, which, for skin dermis tissue in 90% oxygen saturation at red and infrared wavelengths, are 25.62 and 15.68 mm$^{-1}$ respectively. For higher scattering coefficient, the free pathlength between two consecutive scattering events (i.e., $1/\mu_s$) is smaller, thus photons are subjected to more frequent scattering and change of direction. This is the reason red photons appear to be more intensely scattered, whereas the infrared photons travel longer optical paths within the tissue. The negative and positive values of the width of tissue represent the direction of the photons in both sides from the source which is placed at the origin of the system.

The detected reflectance simulated in the similar geometry as described above for a range of arterial oxygen saturation values 10-100% for 660 nm and 940 nm wavelengths are shown in figure 2. Reflectance, which is basically the mean of the remaining weights of the detected photon packets after absorptions in the tissue, is shown to be lower than 1 in all cases, which is expected as the initial
Figure 2. Detected reflectance at range of arterial oxygen saturation values (10-100%) simulated through the dermal tissue slab with a source-detector separation of 6 mm for systole and diastole at 660 nm and 940 nm wavelengths. Each photon packet is 1, and it decays due to multiple absorption events. Diastolic reflectance is always shown to be higher than systolic reflectance. Because of higher volume of blood in tissue during systole than in diastole, the absorption of light in systole is also higher than diastole. Thus, lesser weight of photon is detected in systole compared to diastole. The reflectance varies with arterial oxygen saturation.

Figure 3. Pulse oximeter calibration curve produced by Monte Carlo simulation. The markers show the R values at the arterial oxygen saturation values 10-100%.
increasing arterial oxygen saturation. For lower oxygen saturation, infrared reflectance is higher compared to infrared reflectance. For higher oxygen saturation (>90%), the red reflectance becomes higher compared to the infrared reflectance. The behaviour of the reflectance is dependent on the absorption coefficient values of oxy and deoxyhemoglobin. At 660 nm, the absorption coefficient of oxyhemoglobin is 0.15 mm\(^{-1}\) and that of deoxyhemoglobin in 0.65 mm\(^{-1}\). At 940 nm, the absorption coefficient of oxyhemoglobin is 1.64 mm\(^{-1}\) and that of deoxyhemoglobin in 0.43 mm\(^{-1}\). In low oxygen saturation, the optical properties of deoxyhemoglobin dominate and the dominance of oxyhemoglobin increases with increasing oxygen saturation. This feature results in increasing reflectance at 660 nm and slowly decreasing reflectance at 940 nm, with increasing oxygen saturation.

The ratio of systolic to diastolic reflectances produces the normalized pulsatile intensity. Ratio of red and infrared normalized intensity leads to the ‘ratio of ratios’ R, which is plotted as a function of arterial oxygen saturation in figure 3. It resembles the typical calibration curve of commercial Pulse Oximeters [10].

4. Conclusion
A monolayer pulsatile model for reflectance Pulse Oximetry has been developed using Monte Carlo computational algorithm. The model has been explored for determination of the reflectance (i.e., detected weight of photon packets, which is equivalent to the intensity) at systole and diastole states of the tissue at two most commonly used wavelengths in Pulse Oximeters 660 nm and 940 nm. This model, even though a simplification of a highly heterogeneous tissue structure, demonstrates the feasibility of Monte Carlo method to compute the results which are very close to reality. Future works would be focused on the development of multilayer tissue structure for modelling Pulse Oximetry and Photoplethysmography, and would be applied rigorously for evaluating different parameters such as optical path, penetration depth, detected intensity etc. for different blood volumes and oxygen saturations, and for different sensor geometries (i.e., reflectance and transmittance mode, different source-detector separation in reflectance mode, optical fiber probe as source and detector, different positions and orientations of the source and detector etc.). Such studies are invaluable for the present age of miniaturized and wearable sensor design.

References