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Title: Quantitative Comparison of Analytical Solution and Finite Element Method for Investigation of Near-Infrared Light Propagation in Brain Tissue Model

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Abstract

Introduction: Functional Near-Infrared Spectroscopy (fNIRS) is an imaging method in which light source and detector are installed on the head; consequently, re-emission of light from human skin contains information about cerebral hemodynamic alteration. The spatial probability distribution profile of photons penetrating tissue at a source spot, scattering into the tissue, and being released at an appropriate detector position, represents the spatial sensitivity.

Method: Modeling light propagation in a human head is essential for quantitative near-infrared spectroscopy and optical imaging. The specific form of the distribution of light is obtained using the theory of perturbation. Analytical solution of the perturbative Diffusion Equation (DE) and Finite Element Method (FEM) in a Slab media (similar to the human head) makes it possible to study light propagation due to absorption and scattering of brain tissue.

Results: The simulation result indicates that sensitivity is slowly decreasing in the deep area, and the sensitivity below the source and detector is the highest. The depth sensitivity and computation time of both Analytical and FEM methods are compared. The simulation time of the analytical approach is four orders of magnitude faster than the FEM.

Conclusion: In this paper, an analytical solution and FEM methods performance when applied to the diffusion equation for heterogeneous media with a single spherical defect are compared. The depth sensitivity, along with the computation time of simulation, has been investigated for both methods. For simple and Slab-like human brain models, the analytical solution is the right candidate. Whenever the brain model is sophisticated, it is possible to use FEM methods, but it costs higher computation time.

Keywords: fNIRS, Perturbation theory, Diffusion Equation, Depth sensitivity, Contrast, FEM.

1. Introduction

Functional Near-Infrared spectroscopy is a method for investigating brain activity noninvasively (Berivanlou, Setarehdan, & Noubari, 2014; Ferrari & Quaresima, 2012; Hemmati, Setarehdan, & Noubari, 2012; Rahimpour, Pollonini, Comstock, Balasubramaniam, & Bortfeld, 2020; Scholkmann et al., 2014). This low-cost imaging method has a lot of applications in the field of neuroscience, including infant cerebral hemodynamic monitoring; classification of chronic diseases; stress level, and mental workload assessment; IQ estimation (Dadgostar, Setarehdan, Shahzadi, & Akin, 2018; Firooz & Setarehdan, 2019; Hakimi & Setarehdan, 2018; Jahani, Berivanlou, Rahimpour, & Setarehdan, 2015; Mirbagheri, Hakimi, Ebrahimzadeh, & Setarehdan, 2020b, 2020a; Rahimpour, Dadashi, Soltanian-Zadeh, & Setarehdan, 2017; Rahimpour, Noubari, & Kazemian, 2018). In this imaging method, a light source and detector are installed on the head; consequently, re-emission of light from human skin contains optical information from the human body (Scholkmann et al., 2014). Overall, there are three types of spectroscopy methods from the brain tissue: continuous wave method, time domain, and frequency domain technique (Ferrari & Quaresima, 2012). The first one is simpler and more portable than the other two, and it can wirelessly send hemodynamic information (Chiarelli et al., 2017; Ferrari & Quaresima, 2012; von Lüthmann, Wabnitz, Sander, & Müller, 2017). Studies and results in this work are focused on a CW-fNIRS.

According to Fig. 1 brain, activities are associated with the generation of the action potentials; consequently, the amount of oxygen supply to that part will be raised. It is called the hemodynamic response. A single or multiple channels fNIRS can detect these hemodynamic changes.

Figure 1. It illustrates the procedure of hemodynamic response generation, which can be observed by a single-channel fNIRS instrument.

The single-channel fNIRS helps measure hemodynamic changes based on detected optical modulation. An optical channel is created by setting a light source with a specified distance from the optical receiver. Hemodynamic changes modulate the changes in light received by the detector. It is essential to study the photon propagation profile to obtain the brain tissue's sensitivity of cerebral hemodynamic function. The question is, how long is the depth of penetration in one single channel fNIRS. Another specific issue that arises is that how much the reflectance of the detector is sensitive to depth. The previous study indicates that depths sensitivity decreases exponentially, depending on the source-detector separation (Mirbagheri et al., 2020b; Strangman, Li, & Zhang, 2013).

Analytical methods have been developed earlier to study light emission inside the simple geometry such as slab medium (S R Arridge, Schweiger, Hiraoka, & Delpy, 1993; Simon R Arridge, Cope, & Delpy, 1992; Silvia Carraresi, Shatir, Martelli, & Zaccanti, 2001; Cui & Ostrander, 1992; Haselgrove, Schotland, & Leigh, 1992; Patterson, Chance, & Wilson, 1989; Schweiger, Arridge, & Delpy, 1993). Numerical methods also are used in complex brain models to study light diffusion in tissues (Mansouri, LHuillier, Kashou, & Humeau, 2010; Strangman et al., 2013). The analytical methods take less time calculation than statistical approaches, especially when it comes to investigating the effect of several fNIRS channels on depth sensitivity. It is also possible to evaluate the performance of High-Density (HD) source and detector design topology on several hemodynamic reconstructions by using an analytical approach (Borjkhani & Setarehdan, 2020). In this paper, using a perturbative Diffusion Equation, the light emission profile for a channel is studied. The photon beam propagation path into the tissue is investigated for both the perturbation theory on Diffusion Equation (DE) (S Carraresi, Shatir, Martelli, & Zaccanti, 2001) and FEM. The detector's sensitivity to hemodynamic changes can be determined with the knowledge of the pathway of photons propagation. Both methods improve our understanding of the emission of photons into the human brain. The benefits and drawbacks of each approach will be discussed in this article.

The next section will describe the theory and mathematics governing the model. All the equations are solved in a medium like the human brain for both Analytical and FEM methods. In the third section, the photon's contrast in different X, Y-plane, and at different depths are simulated. The final part will discuss the quantitative comparison between these two methods and further address their benefits and limitations.

2. Material and Methods

2.1. Analytical Solution

To study the transmission and reflectance of the light between pairs of source and detector concerning the configuration of the source and detectors on the surface of the medium and also to find out the three-dimensional distribution of photon inside it, an appropriate model of photon transport need to be used (Sassaroli, Martelli, & Fantini, 2006). The models that have been

developed for this task are based on the radiative transfer theory. The derivatives of the Radiative Transfer Equation (RTE) are stochastic or deterministic. There is no analytical answer to solve this equation. Therefore, simpler models of this equation are extracted. With some assumptions and simplification, Diffusion Equation (DE) is derived from RTE (Martelli, Del Bianco, Ismaelli, & Zaccanti, 2010). DE is a practical mode, and there is an analytical solution for it. The DE solution should be applied to inhomogeneous media similar to brain tissue properties. The photons' intensity that undergoes many scattering events and being detected by the detector is called reflectance. Reflectance can be obtained by solution of DE in Slab geometry. The optical properties of the Slab assumed to be: $\mu_a = 0.017\text{mm}^{-1}$ and $\mu_s = 1.2\text{mm}^{-1}$ and $S = 40\text{mm}$ and refractive index $n_r = 1.4$.

Figure 2. This figure illustrates the slab geometry and location of the source $\vec{r}_0$ and detector $\vec{r}_3$ and inclusion $\vec{r}_2$.

In an environment modeled with optical properties identical to the human brain (Shown in Fig.2), an optical source in the location (x_0, y_0, z_0) and a detector in position (x_3, y_3, z_3) are placed at a given distance from the source. By placing an inclusion inside the mediums in (x_2, y_2, z_2) , the reflectance concerning the inclusion is calculated. The perturbed reflectance due to inclusion inside medium can be obtained by (S Carraresi et al., 2001):

$$R^{pert}(\rho) = R^0(\rho) + \delta R^a(\rho) + \delta R^D(\rho) \quad (1)$$

where, $R^0(\rho)$ is the reflectance inside homogeneous media, $\delta R^a(\rho)$ and $\delta R^D(\rho)$ are absorption and scattering effects of the inhomogeneity sphere, respectively.

$$R^0(\rho) = \int_0^{+\infty} R(\rho, t) dt = -\frac{1}{4\pi} \sum_{m=-\infty}^{\infty} \left(\begin{aligned} & z_{3m}(\rho^2 + z_{3m}^2)^{-3/2} \times \left\{ 1 + \left[\frac{\mu_a(\rho^2 + z_{3m}^2)}{D} \right]^{1/2} \right\} \\ & \times \exp \left\{ - \left[\frac{\mu_a(\rho^2 + z_{3m}^2)}{D} \right]^{1/2} \right\} - z_{4m}(\rho^2 + z_{4m}^2)^{-3/2} \\ & \times \left\{ 1 + \left[\frac{\mu_a(\rho^2 + z_{4m}^2)}{D} \right]^{1/2} \right\} \times \exp \left\{ - \left[\frac{\mu_a(\rho^2 + z_{4m}^2)}{D} \right]^{1/2} \right\} \end{aligned} \right) \quad (2)$$

where $z_{3m} = -2ms - 4mz_e - z_s$, $z_{4m} = -2ms - 4mz_e + 2z_e + z_s$ and "s" is the thickness of the Slab and $\rho = \sqrt{(x_3 - x_0)^2 + (y_3 - y_0)^2}$ is the distance between source and detector. μ_a is the absorption coefficient, and D is the diffusion coefficient. In steady-state condition, the perturbation for reflectance due to absorption of the inhomogeneity for the channel is:

$$\delta R^a(\rho) = -\frac{1}{(4\pi)^2 D} \times \sum_{m=-\infty}^{\infty} \sum_{\eta=-\infty}^{\infty} \int_{Vi} d^3 \vec{r}_2 \delta \mu_a(\vec{r}_2) \times \left(\begin{aligned} & z_{23\eta}' \frac{1 + \mu_{eff} \rho_{23\eta}^{+'}}{(\rho_{23\eta}^{+'})^3} \left\{ \frac{\exp[-\mu_{eff}(\rho_{12m}^{+'} + \rho_{23\eta}^{+'})]}{\rho_{12m}^{+'}} - \frac{\exp[-\mu_{eff}(\rho_{12m}^{+'} + \rho_{23\eta}^{+'})]}{\rho_{12m}^{+'}} \right\} \\ & - z_{23\eta}' \frac{1 + \mu_{eff} \rho_{23\eta}^{-'}}{(\rho_{23\eta}^{-'})^3} \left\{ \frac{\exp[-\mu_{eff}(\rho_{12m}^{+'} + \rho_{23\eta}^{-'})]}{\rho_{12m}^{+'}} - \frac{\exp[-\mu_{eff}(\rho_{12m}^{+'} + \rho_{23\eta}^{-'})]}{\rho_{12m}^{+'}} \right\} \end{aligned} \right) \quad (3)$$

Where $\rho = \sqrt{(x_3 - x_0)^2 + (y_3 - y_0)^2}$, $z_e = 2AD$, D is the diffusion coefficient, and A is dependent on the refractive index:

$$A = 504.332889 - 2641.00214n + 5923.699064n^2 - 7376.355814n^3 + 5507.53041n^4 - 2463.357945n^5 + 610.956547n^6 - 64.8047n^7 \text{ for } n > 1 \quad (4)$$

$$A = 3.084635 - 6.531194n + 8.357854n^2 - 5.0082751n^3 + 1.171382n^4 \text{ for } n \leq 1 \quad (5)$$

And also, h and w functions are given (S Carraresi et al., 2001):

$$w(x, y, \mu_{eff}) = \frac{1 + \mu_{eff}x}{x^2} \left[\frac{3 + 3\mu_{eff}y + \mu_{eff}^2 y^2}{y^4} \right] \exp[-\mu_{eff}(x + y)] \quad (6)$$

$$h(x, y, \mu_{eff}) = \frac{1 + \mu_{eff}x}{x^3} \left[\frac{1 + \mu_{eff}y}{y^3} \right] \exp[-\mu_{eff}(x + y)] \quad (7)$$

where $\mu_{eff} = \sqrt{\mu_a/D} = \sqrt{3\mu_a\mu'_s}$ is the effective attenuation coefficient.

The perturbed reflectance in the channel is obtained by sweeping the inhomogeneity in three-dimensional space. The perturbed reflectance due to scattering is considered to be constant for the sake of simplicity. The spatial probability distribution profile of photons penetrating tissue at a source spot, scattering into the tissue, and being released at an appropriate detector position, represents the spatial sensitivity.

2.2. Finite Element Method (FEM)

One of the numerical approaches for the solution of DE in the slab medium is FEM. The optical properties of the medium, in this case, is considered the same as section 2.1. The dimension of the Slab is $120mm \times 120mm \times 40mm$. The source and detector are placed in $(40mm, 60mm, 0)$ and $(80mm, 60mm, 0)$, respectively. The distance between them is 40mm same as the previous section. The inclusion with only a 5-6% change in optical properties of the background medium is inserted under the source and detector's surface and inside the medium. The geometry and mesh for the FEM solution presented in Fig. 3.

Figure 3. (a) Indicates the geometry of the medium. (b) Represents the fine mesh for the Slab geometry, which is indicated in (a).

The FEM is applied to the steady-state diffusion equation:

$$D\nabla^2\phi(\vec{r}) - \mu_a\phi(\vec{r}) = f(\vec{r}) \quad \nabla = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right] \quad (8)$$

where $\phi(\vec{r})$ is the fluence rate, which is a scalar intensity (in units of $\frac{W}{m^2}$), represents the power of light radiating radially per area at position $\vec{r}$ and $f(\vec{r})$ indicates the power per area from source element at position $\vec{r}$ (Wheelock, Culver, & Eggebrecht, 2019). The geometry in Fig. 3(a) is discretized into voxels in Fig.3 (b). Then the equation (8) is solved for each voxel to calculate the FEM method's solution. The size of the geometry elements controls the size of voxels to reduce the computation time of FEM. Since the size of the source, detector, and inclusion are small, then the voxels beside them are small and grow more extensive in the far distance from them. The depth sensitivity for the FEM method is calculated using the defined sensitivity equation:

$$Sensitivity(z) = \frac{\Delta R(\vec{r}_D, \vec{r}_p, \mu_{a2}) - \Delta R(\vec{r}_D, \vec{r}_p, \mu_{a1})}{(\mu_{a2} - \mu_{a1}) \cdot V_i \times R_0(\vec{r}_D)} \quad (9)$$

where $\Delta R(\vec{r}_D, \vec{r}_p, \mu_a) = \iint_0^{2\pi} \Delta \phi(\vec{r}_D, \mu_a) d\theta dr$, which is the integral of total power reflected the detector area in existing of the perturbation in position $\vec{r}_p$ with μ_a absorption coefficient. And $R_0(\vec{r}_D) = \iint_0^{2\pi} \Delta \phi_0(\vec{r}_D) d\theta dr$ is the integral of the total power reflected in the detector area inhomogeneous medium without any inclusion. V_i refers to the volume of the perturbation. It is better to note that the shape and size of the source and detector are considered a circle with a 1.5mm radius, and the inclusion is a cubic element with a volume of $2mm \times 2mm \times 2mm$.

The next section described the simulation results of the spatial sensitivity for both Analytical and FEM approaches.

3. Results

For an analytical case, the inclusion has been moved under the source and detector surface to measure the relative perturbation $\delta R^a/R^0$ (Contrast) Versus Y-plane. The result of this simulation has been shown in Fig.3 for Y=2mm, Y=3mm, Y=4mm, and Y=5mm. The result of this simulation indicates that sensitivity is slowly decreasing, and on the other hand, the sensitivity below the source and detector is the highest. Concerning Fig. 4(a), the dominant pathway of photons is a banana shape. According to Fig. 4(b), Fig. 4(c), and Fig. 4(d), as the inclusion moves away from the Y=0, the sensitivity is decreasing.

The same procedure is repeated in Fig.5 for Z-plane to achieve an image for spatial sensitivity in depth. According to this simulation, the sensitivity in Fig.5 (a) is higher (in Z=10mm) compared to Fig. 5(b), Fig. 5(c), and Fig. 5(d).

Figure 4. $\delta R^a / R^a$ (Contrast) versus Y-plane in Y=2mm, 3mm, 4mm, and 5mm for optical source in the location (0, 0, 0) and a detector in position (40, 0, 0). (a) Represents the spatial sensitivity profile in Y=2mm. (b), (c) and (d) illustrate reduced sensitivity concerning separation from Y=2mm, in Y=3mm, Y=4mm, and Y=5mm, respectively.

Figure 5. $\delta R^a/R^a$ (Contrast) versus Z-plane in Z=10mm, 12.5mm, 15mm, and 17.5mm for optical source in the location (0, 0, 0) and a detector in position (40, 0, 0). (a) Indicates the spatial sensitivity profile in Z=10mm. (b), (c) and (d) represent reduced sensitivity concerning separation from Z=10mm, in Z=12.5mm, Z=15mm, and Z=17.5mm, respectively.

The depth sensitivity of both Analytical and FEM is calculated for the same Slab geometry with the same optical properties. The result of the comparison of sensitivity between these methods is shown in Fig. 6. Regarding this figure, the depth sensitivity reduced gradually in-depth, and the shape of sensitivity for both approaches is almost identical. The depth sensitivity depends on the geometry and size of the source and detector and perturbation size. The volume of perturbation and its associate absorption coefficient directly impact the depth sensitivity. The radius of the

source and detector for FEM simulation is 1.5mm. In the FEM approach, the sensitivity is calculated according to equation (9). The depth sensitivity of analytical and FEM method for source and detector distance of 40mm is also compared in Fig. 7 (in this comparison, the amount of perturbation for both approaches is $\delta\mu_a \cdot V_i = 1\text{mm}^2$). Finally, Table 1 summarizes the results of the comparison between the two methods. Both of them take advantage of the simple diffusion approximation of RTE. However, there is a considerable difference between computation time. MATLAB and COMSOL Multiphysics are the simulation environments for analytical and FEM simulations, respectively. The software is running on a laptop computer with an Intel Core-i5 processor and 4GB RAM.

Figure 6. (a), (b), (c), and (d) Represents the depth sensitivity of the Analytical and FEM in Z=-2mm, Z=-4mm, Z=-8mm, and Z=-16mm, respectively.

Table 1. Quantitative comparison between Analytical and FEM solution of DE

Simulation methods	Mathematical equations	Computation time (s)	Depth sensitivity equation	Simulation Environment	The solution in complex geometries
Analytical	DE	0.038	$\delta R^a / R^0$	MATLAB	No
FEM	DE	380-400	$\frac{\Delta R(\vec{r}_D, \vec{r}_p, \mu_{a2}) - \Delta R(\vec{r}_D, \vec{r}_p, \mu_{a1})}{(\mu_{a2} - \mu_{a1}) \cdot V_i \times R_0(\vec{r}_D)}$	COMSOL and MATLAB Live Link	Yes

Figure 7. (a) Represents the calculated depth sensitivity for the analytical method. (b) Illustrates the depth sensitivity calculated by the FEM method. In both approaches, the amount of perturbation is $\delta\mu_a \cdot V_i = 1mm^2$ and the distance between source and detector is 40mm.

Discussion

In this paper, perturbation theory is applied for the analytical solution of the DE in slab media based on the method in (S Carraresi et al., 2001). The solution of FEM is applied to the diffusion equation and the results of depth sensitivity compared to both methods. In the FEM solution, the volume and shape of the source, detector, and perturbation can be changed. Even it is possible to calculate the solution for complex geometries (Wheelock et al., 2019).

Using both simulation approaches, one can obtain the trajectory of photon propagation received by the optical detector. Although the FEM can be applied to sophisticated geometries like the human brain and several options to study the effect of source and detector size on simulation, the computation time of FEM is four orders of magnitude higher than Analytical simulation. One of the significant contributions of this investigation is to compare the computation time of each method.

It is assumed that the human brain is only one layer, while realistic results can be obtained by taking several layers (since, in reality, the head model has several layers). The perturbation theory's accuracy in the article (Silvia Carraresi et al., 2001) is compared with the MC analysis results. There is a good agreement between the solution of perturbative DE and MC simulation. We can examine the depth of penetration and the photon propagation's shape by regulating the distance between the source and the light detector. This study would help fNIRS researchers design a better measurement setup in the instrumentation part and reconstruct the hemodynamic response concerning spatial sensitivity.

The quantitative comparison concludes that the elapsed simulation time in FEM is higher than analytical. When the number of simulated channels exceeds more than 100 channels, the simulation time will change from several minutes to several hours. It is recommended to use the analytical method when the geometry of the head model is simple. For complex geometries, the FEM would be a suitable option despite the computation time challenge. The calculated depth sensitivity for both methods is almost identical. It is expected because, in both procedures, the head model's optical properties and geometry are similar, and diffusion approximation has been used for both techniques.

The introduced strategies can be applied for the study of light-tissue interaction and simulation of synthetic fNIRS channels (Bonomini et al., 2015; Borjkhani & Setarehdan, 2020; Torricelli et al., 2005). The analytical and FEM results will be compared with laboratory results in future work by implementing a near-infrared spectroscopy system and liquid phantom.

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