Modeling hemoglobin at optical frequency using the unconditionally stable fundamental ADI-FDTD method

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Abstract: This paper presents the modeling of hemoglobin at optical frequency (250 nm - 1000 nm) using the unconditionally stable fundamental alternating-direction-implicit finite-difference time-domain (FADI-FDTD) method. An accurate model based on complex conjugate pole-residue pairs is proposed to model the complex permittivity of hemoglobin at optical frequency. Two hemoglobin concentrations at 15 g/dL and 33 g/dL are considered. The model is then incorporated into the FADI-FDTD method for solving electromagnetic problems involving interaction of light with hemoglobin. The computation of transmission and reflection coefficients of a half space hemoglobin medium using the FADI-FDTD validates the accuracy of our model and method. The specific absorption rate (SAR) distribution of human capillary at optical frequency is also shown. While maintaining accuracy, the unconditionally stable FADI-FDTD method exhibits high efficiency in modeling hemoglobin.

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1. Introduction

The information on optical properties of human blood is crucial for many medical applications. In particular, the hemoglobin in red blood cells plays an important role by transporting oxygen throughout the human body. Past literatures have successfully determined the molar extinction coefficient [1–7] of hemoglobin at optical frequency. The real part of its complex refractive index has also been found using transmittance and reflectance measurements [8–10]. With such knowledge on the complex refractive index, a better understanding of the interaction of light with the biological media is greatly desired. Owing to this, the finite-difference time-domain (FDTD) method [11, 12] has been widely used for solving electromagnetic problems and modeling electromagnetic wave propagation in various media. Unfortunately, the usage of such explicit FDTD method is limited by the fact that its time step is restricted by the Courant-Friedrich-Lewy (CFL) condition, given below as

$$\Delta t \leq \frac{\mu \varepsilon}{\Delta x^2 + \Delta y^2 + \Delta z^2}$$

where $\varepsilon$ and $\mu$ are the permittivity and permeability of the media, respectively. $\Delta t$, $\Delta x$, $\Delta y$ and $\Delta z$ are the time step and spatial steps in $x$, $y$ and $z$-directions, respectively. The above equation...
which sets the numerical stability bound for classical FDTD was first derived and published in [13]. Note that if the spatial steps are small, this restriction may result in undesirably long simulation time.

The conventional alternating-direction-implicit finite-difference time-domain (ADI-FDTD) method [14,15], on the other hand, has unconditional stability feature where the time step is no longer restricted by the CFL stability criterion. This has circumvented the above limitation in its own right. However, due to the fact that the algorithm is implicit in nature, its implementation is complicated. Not only are there tri-diagonal systems that need to be solved, the right-hand-side (RHS) of each equations involve many update coefficients and field variables, which calls for considerable arithmetic operations and memory indexing. Recently, these overheads has been overcome by the introduction of the fundamental alternating-direction-implicit finite-difference time-domain (FADI-FDTD) method [16,17]. In FADI-FDTD, its algorithm is included within a family of fundamental implicit schemes, which feature similar fundamental updating structures that are in simplest forms with most efficient matrix-operator-free RHS. This leads to substantial reduction in arithmetic operations and memory indexing. Nevertheless, while the evolution of computational electromagnetic in time domain from explicit FDTD method to FADI-FDTD has been encouraging, there is still a lack of appropriate complex permittivity models for biological media (in this case, hemoglobin) at optical frequency. Even then, the implementation of such appropriate complex permittivity models into the FADI-FDTD is also highly sought after.

In this paper, we seek to address the aforementioned problems and bridge the necessary gaps. First, we propose a model based on complex conjugate pole-residue pairs to describe the electrical behaviour of hemoglobin, where it is fitted against the complex refractive index data. Once an accurate model is found, it is incorporated into FADI-FDTD method for solving electromagnetic problems involving light interactions with biological media. Finally, some numerical examples are provided to validate the proposed method and to demonstrate some electromagnetic wave interactions with human blood at optical frequency.

2. Complex relative permittivity model for hemoglobin

2.1. Complex refractive index data

We first denote the wavelength dependent complex refractive index of hemoglobin as

\[ n(\lambda) = n_r(\lambda) - jk(\lambda) \]  (2)

where \( j = \sqrt{-1} \), \( n_r \) is the real part of the refractive index and \( k \) is known as the extinction coefficient which is related to the absorption coefficient, \( \mu_a \) of the medium by

\[ k = \frac{\mu_a \lambda}{4\pi} \]  (3)

with \( \lambda \) being the free space wavelength. Note that the convention of time dependence \( e^{j\omega t} \) is used throughout the paper. \( k \) is always positive to yield negative imaginary part in Eq. (2) for losses or absorption in the media.

We make use of the tabulated molar extinction coefficient, \( e \), data in [5]. The absorption coefficient of various hemoglobin concentrations can be obtained from the molar extinction coefficient by means of the following relation:

\[ \mu_a = \ln(10) \times e \times \frac{C}{64500} \]  (4)

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where $C$ is the hemoglobin concentration in g/L. Note that $e$ has the unit of L mol$^{-1}$ cm$^{-1}$ or M$^{-1}$ cm$^{-1}$ and 64500 is the gram molecular weight of hemoglobin in g/mol. Once the absorption coefficient is obtained, the imaginary part of the complex refractive index can be extracted through Eq. (3). On the other hand, the real part of the complex refractive index of hemoglobin at optical frequency has been determined and it is found to be related to the real part of the complex refractive index of water through a model function proposed in [10] as

$$n_r = n_{wr} (\beta c + 1)$$  \hspace{1cm} (5)$$

where $n_{wr}$ is the real part of complex refractive index of water and $c$ is the hemoglobin concentration in g/dL (1 dL = 0.1 L). $\beta$ is the specific refractive increment which is also wavelength dependent and tabulated in [10].

Therefore, using Eq. (4) and Eq. (5), the complex refractive index of hemoglobin at optical frequency can be extracted for various concentrations conveniently. Figure 1 plots the (a) real part of complex refractive index, $n_r$, and (b) extinction coefficient, $k$, respectively, versus wavelength, $\lambda$, for various hemoglobin concentrations. It can be seen that $n_r$ increases with higher hemoglobin concentration across all wavelengths. The same also holds true for $k$, which indicates that higher hemoglobin concentration results in higher absorption (more loss). Another point to note is that when the hemoglobin concentration is at 0 g/dL, its $n_r$ corresponds to that of water [18]. At this 0 g/dL concentration the $k$ value is also reduced to zero. This is based on the fact that water has a “transparency window” at the visible light and near infrared region, in which it has negligible absorption or losses.

2.2. Complex conjugate pole-residue pair model

In electromagnetic analysis, we are more interested in the complex relative permittivity rather than the refractive index. The complex relative permittivity is related to the refractive index by

$$\varepsilon(\omega) = n(\omega)^2$$

$$= n_r(\omega)^2 - k(\omega)^2 - j2n_r(\omega)k(\omega)$$  \hspace{1cm} (6)$$
activity or complex refractive index, we assume that they all share the same poles. Since all hemoglobin concentrations have rather the same trends of complex relative permittivity, the complex relative permittivity data extracted from Eq. (6) using the methodology detailed in [19] to obtain the values of \( \varepsilon_\infty \) can then be extracted using Eq. (6) from the values of \( n_\varepsilon \) and \( k_\varepsilon \) earlier. We now propose a complex relative permittivity model for hemoglobin. It can be described based on complex conjugate pole-residue pairs as follows:

\[
\varepsilon(\omega) = \varepsilon_\infty + \sum_p \left( \frac{r_p}{j\omega - a_p} + \frac{r_p^*}{j\omega - a_p^*} \right)
\]

(7)

where \( \varepsilon_\infty \) is the relative permittivity at infinite frequency, \( a_p \) and \( r_p \) are the \( p \)-th pole and residue, respectively.

The model based on complex conjugate pole-residue pairs in Eq. (7) is then fitted against the complex relative permittivity data extracted from Eq. (6) using the methodology detailed in [19] to obtain the values of \( \varepsilon_\infty, a_p \) and \( r_p \). The values are fitted within the frequency range of 300 THz to 1200 THz (250 nm-1000 nm wavelength). In practical medical applications we are often interested in only two hemoglobin concentrations. The first one is the hemoglobin concentration in erythrocytes (red blood cells), which is also commonly known as mean corpuscular hemoglobin concentration (MCHC). Typical MCHC value for a healthy adult is around 33 g/dL. The second one is the overall hemoglobin concentration in human blood, which consists of not only erythrocytes, but also leukocytes (white blood cells), thrombocytes (platelets) and plasma. The overall hemoglobin concentration for a healthy adult is around 15 g/dL, and this corresponds to hematocrit (which is the proportion of blood volume that is occupied by red cells) of around 45 percent. It is found that using 6 pairs (order 12) of complex conjugate pole and residue pairs can sufficiently fit the experimental data. The values of \( \varepsilon_\infty, a_p \) and \( r_p \) for hemoglobin concentrations of 15 g/dL and 33 g/dL are provided in Tables 1 and 2, respectively.

Since all hemoglobin concentrations have rather the same trends of complex relative permittivity or complex refractive index, we assume that they all share the same poles \( a_p \). That is,

### Table 1. Fitted Values of \( a_p, r_p \) and \( \varepsilon_\infty \) for Hemoglobin Concentration of 15 g/dL

| \( p \) | \( a_p \) | \( r_p \) |
|-------|-------|-------|
| 1     | \(-3.1751 \times 10^{14} + j2.4717 \times 10^{15}\) | \(-2.0191 \times 10^{10} + j1.6882 \times 10^{10}\) |
| 2     | \(-7.1750 \times 10^{13} + j3.2611 \times 10^{15}\) | \(1.1223 \times 10^{11} - j2.0688 \times 10^{11}\) |
| 3     | \(-3.6183 \times 10^{13} + j3.4679 \times 10^{15}\) | \(3.6477 \times 10^{10} - j9.6911 \times 10^{10}\) |
| 4     | \(-1.4538 \times 10^{14} + j4.5108 \times 10^{15}\) | \(7.1508 \times 10^{14} - j3.6455 \times 10^{12}\) |
| 5     | \(-5.5353 \times 10^{14} + j5.3385 \times 10^{15}\) | \(2.0872 \times 10^{14} - j2.2396 \times 10^{14}\) |
| 6     | \(-3.2153 \times 10^{13} + j9.5959 \times 10^{15}\) | \(-4.2183 \times 10^{14} - j3.9864 \times 10^{14}\) |

\( \varepsilon_\infty = 1.7844 \)

### Table 2. Fitted Values of \( a_p, r_p \) and \( \varepsilon_\infty \) for Hemoglobin Concentration of 33 g/dL

| \( p \) | \( a_p \) | \( r_p \) |
|-------|-------|-------|
| 1     | \(-3.1751 \times 10^{14} + j2.4717 \times 10^{15}\) | \(-3.8401 \times 10^{10} + j5.8207 \times 10^{10}\) |
| 2     | \(-7.1750 \times 10^{13} + j3.2611 \times 10^{15}\) | \(2.8608 \times 10^{11} - j5.0495 \times 10^{11}\) |
| 3     | \(-3.6183 \times 10^{13} + j3.4679 \times 10^{15}\) | \(1.0080 \times 10^{11} - j2.2246 \times 10^{11}\) |
| 4     | \(-1.4538 \times 10^{14} + j4.5108 \times 10^{15}\) | \(1.6344 \times 10^{14} - j8.0730 \times 10^{12}\) |
| 5     | \(-5.5353 \times 10^{14} + j5.3385 \times 10^{15}\) | \(3.6171 \times 10^{14} - j5.2711 \times 10^{14}\) |
| 6     | \(-3.2153 \times 10^{13} + j9.5959 \times 10^{15}\) | \(-1.4155 \times 10^{14} - j4.5947 \times 10^{14}\) |

\( \varepsilon_\infty = 1.8994 \)
Fig. 2. (a) Real part, $\varepsilon_r$, and (b) imaginary part, $\varepsilon_i$, of complex relative permittivity versus wavelength, $\lambda$: model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. A good fit is observed between our proposed model and experimental data across all wavelengths.

Fig. 3. Absorption coefficient, $\mu_a$, versus wavelength, $\lambda$: model and experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL.

once the poles are identified for one hemoglobin concentration, they can be reused as poles of other hemoglobin concentrations. Only the new values of residues are calculated to avoid tedious searching of new poles.

Using the values provided in Tables 1 and 2, we plot the real and imaginary part of the fitted model based on complex conjugate pole-residue pairs and compare them with the experimental data obtained in the previous subsection. Figure 2 plots the (a) real and (b) imaginary parts of the complex relative permittivity versus wavelength for both our model and experimental data. The absorption coefficient is then plotted in Fig. 3. It is evident that our model in Eq. (7), along with the values given in Tables 1 and 2, provide a good fit to the experimental data for hemoglobin concentrations of 15 g/dL and 33 g/dL. The proposed model is thus expected to describe the electromagnetic behaviour of hemoglobin accurately in the wavelength regions of
250 nm to 1000 nm.

3. Implementation using fundamental ADI-FDTD (FADI-FDTD) method

To incorporate the hemoglobin model into FADI-FDTD update equations, we first write down the Maxwell’s curl equations as

\[ \nabla \times \mathbf{H}(t) = \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \varepsilon_0 \sum_p \frac{g^{-1}}{j \omega} \left\{ j \omega \left( \frac{r_p}{j \omega - a_p} + \frac{r^*_p}{j \omega - a^*_p} \right) \mathbf{E}(\omega) \right\} \]

\[ = \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_p \left( \mathbf{J}_p(t) + \mathbf{J}_p^*(t) \right) \tag{8a} \]

\[-\nabla \times \mathbf{E}(t) = \mu_0 \mu_{\infty} \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \mu_0 \sum_p \frac{g^{-1}}{j \omega} \left\{ j \omega \left( \frac{q_p}{j \omega - b_p} + \frac{q^*_p}{j \omega - b^*_p} \right) \mathbf{H}(\omega) \right\} \]

\[ = \mu_0 \mu_{\infty} \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \sum_p \left( \mathbf{M}_p(t) + \mathbf{M}_p^*(t) \right) \tag{8b} \]

where \( \varepsilon_0 \) and \( \mu_0 \) are the permittivity and permeability in free space and \( \sigma \) and \( \sigma^* \) are the electric and magnetic conductivities, respectively. For completeness, we have also included the implementation of magnetic complex conjugate pole-residue pairs model with permeability at infinite frequency \( \mu_{\infty} \). \( p \)-th pole \( b_p \) and residue \( q_p \). The symbol \( g^{-1} \) denotes inverse Fourier transform operation and two sets of auxiliary variables \( \mathbf{J}_p \) and \( \mathbf{J}_p^* \), \( \mathbf{M}_p \) and \( \mathbf{M}_p^* \) have been introduced. These two sets of variables are related to electric field \( \mathbf{E} \) and magnetic field \( \mathbf{H} \) by the following equations:

\[ \frac{\partial}{\partial t} \mathbf{J}_p(t) - a_p \mathbf{J}_p(t) = \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} \mathbf{E}(t) \tag{9a} \]

\[ \frac{\partial}{\partial t} \mathbf{J}_p(t) - a^*_p \mathbf{J}_p(t) = \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} \mathbf{E}(t) \tag{9b} \]

\[ \frac{\partial}{\partial t} \mathbf{M}_p(t) - b_p \mathbf{M}_p(t) = \mu_0 q_p \frac{\partial}{\partial t} \mathbf{H}(t) \tag{10a} \]

\[ \frac{\partial}{\partial t} \mathbf{M}_p(t) - b^*_p \mathbf{M}_p(t) = \mu_0 q^*_p \frac{\partial}{\partial t} \mathbf{H}(t). \tag{10b} \]

It is worth noting that since \( \mathbf{E}(t) \) and \( \mathbf{H}(t) \) are always of real value, \( \mathbf{J}(t) = \mathbf{J}^*(t) \) and \( \mathbf{M}(t) = \mathbf{M}^*(t) \) always hold and Eq. (8) can be simplified to

\[ \nabla \times \mathbf{H}(t) = \varepsilon_0 \varepsilon_{\infty} \frac{\partial}{\partial t} \mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_p 2 \text{Re} \left\{ \mathbf{J}_p(t) \right\} \tag{11a} \]

\[ -\nabla \times \mathbf{E}(t) = \mu_0 \mu_{\infty} \frac{\partial}{\partial t} \mathbf{H}(t) + \sigma^* \mathbf{H}(t) + \sum_p 2 \text{Re} \left\{ \mathbf{M}_p(t) \right\}. \tag{11b} \]

Therefore, only variables \( \mathbf{J} \) and \( \mathbf{M} \) are needed to be solved. We then discretize Eq. (9a) and Eq. (10a) in time using central difference approximation (at time index \( n = 1/4 \)) to yield

\[ \mathbf{J}^{n+1/2} = \frac{1 + a_p \Delta t}{1 - a_p \Delta t} \mathbf{J}^n_p + \frac{r_p}{1 - a_p \Delta t} \left( \mathbf{E}^{n+1/2}_p - \mathbf{E}^n_p \right) = k_{1p} \mathbf{J}^n_p + k_{2p} \left( \mathbf{E}^{n+1/2}_p - \mathbf{E}^n_p \right) \tag{12a} \]

\[ \mathbf{M}^{n+1/2} = \frac{1 + b_p \Delta t}{1 - b_p \Delta t} \mathbf{M}^n_p + \frac{q_p}{1 - b_p \Delta t} \left( \mathbf{H}^{n+1/2}_p - \mathbf{H}^n_p \right) = l_{1p} \mathbf{M}^n_p + l_{2p} \left( \mathbf{H}^{n+1/2}_p - \mathbf{H}^n_p \right). \tag{12b} \]
The time step used in the central difference approximation is $\Delta t/2$ because FADI-FDTD method has two substeps with each substep having time step of $\Delta t/2$. Note that apart from the central difference approximation, the corrected impulse invariance method in Z-transform theory [20] can also be utilized. Along with Eq. (12), we first discretize Eq. (11) into ADI-FDTD of conventional form. The $E_x$ and $H_z$ components of first substep is written as

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} \left( d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} \right) = c_1 E_x^n - c_2 \frac{\partial}{\partial z} H_y^n - c_2 \sum_p \text{Re} \left\{ (1+k_1 p) J_{zp}^n \right\}$$

(13a)

$$H_z^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} = d_1 H_z^n - d_2 \frac{\partial}{\partial z} E_x^n - d_2 \sum_p \text{Re} \left\{ (1+k_1 p) M_{zp}^n \right\}$$

(13b)

where

$$c_1 = \frac{1 - \sigma_1 \Delta t}{4\mu_0\epsilon_0} + \frac{\Delta t}{4\mu_0\epsilon_0} \sum_p 2 \text{Re}(k_2 p),$$

$$c_2 = \frac{1 + \sigma_1 \Delta t}{2\mu_0\epsilon_0} + \frac{\Delta t}{2\mu_0\epsilon_0} \sum_p 2 \text{Re}(k_2 p),$$

$$d_1 = \frac{1 - \sigma_1 \Delta t}{4\mu_0\epsilon_0} + \frac{\Delta t}{4\mu_0\epsilon_0} \sum_p 2 \text{Re}(l_2 p),$$

$$d_2 = \frac{1 + \sigma_1 \Delta t}{2\mu_0\epsilon_0} + \frac{\Delta t}{2\mu_0\epsilon_0} \sum_p 2 \text{Re}(l_2 p).$$

(14a)

(14b)

To solve for $E_x$, we need to substitute Eq. (13b) into Eq. (13a) to obtain the implicit electric field update equation as

$$E_x^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} \left( d_2 \frac{\partial}{\partial y} E_x^{n+\frac{1}{2}} \right) = c_1 E_x^n - c_2 \frac{\partial}{\partial z} H_y^n - c_2 \sum_p \text{Re} \left\{ (1+k_1 p) J_{zp}^n \right\} + c_2 \frac{\partial}{\partial y} (d_1 H_z^n - d_2 \frac{\partial}{\partial z} E_x^n - d_2 \sum_p \text{Re} \left\{ (1+l_1 p) M_{zp}^n \right\}).$$

(15)

When the spatial differential operators are approximated using the second-order central differencing operated on a standard Yee’s cell [11], the electric field components can be obtained by solving a set of tridiagonal matrices.

The full update equations of conventional ADI-FDTD can be summarized in compact matrix form (in two substeps) as

$$(I_{18} - D_2 A + F_r) u^{n+\frac{1}{2}} = (D_1 + D_2 B + F_r) u^n + D_2 s^{n+\frac{1}{2}}$$

(16a)

$$(I_{18} - D_2 B + F_r) u^{n+1} = (D_1 + D_2 A + F_r) u^{n+\frac{1}{2}} + D_2 s^{n+\frac{1}{2}}$$

(16b)

where

$$u = [E_x, E_y, E_z, H_x, H_y, H_z, J'_x, J'_y, J'_z, J''_x, J''_y, J''_z, M'_x, M'_y, M'_z, M''_x, M''_y, M''_z]^T$$

(17)

$$s = [-s_{ex}, -s_{ey}, -s_{ez}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]^T$$

(18)

$$A = \begin{bmatrix} O_3 & K_1 & O_3 & O_3 & O_3 & O_3 \\ K_2 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ \end{bmatrix}, \quad B = \begin{bmatrix} O_3 & -K_2 & O_3 & O_3 & O_3 & O_3 \\ -K_1 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ O_3 & O_3 & O_3 & O_3 & O_3 & O_3 \\ \end{bmatrix}$$

(19)
\[ \mathbf{K}_1 = \begin{bmatrix} 0 & 0 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & 0 \\ 0 & \frac{\partial}{\partial x} & 0 \end{bmatrix}, \quad \mathbf{K}_2 = \begin{bmatrix} 0 & 0 & \frac{\partial}{\partial z} \\ 0 & 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & 0 & 0 \end{bmatrix} \] (20)

\[ \mathbf{D}_1 = \text{diag}(c_1, c_1, c_1, d_1, d_1, d_1, k_1', k_1', k_1', k_1', k_1', l_1', l_1', l_1', l_1') \] (21)

\[ \mathbf{D}_2 = \text{diag}(c_2, c_2, c_2, d_2, d_2, d_2, 0, 0, 0, 0, 0, 0, 0, 0, 0) \] (22)

\[ \mathbf{F}_l = \begin{bmatrix} \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix} \] (23)

\[ \mathbf{F}_r = \begin{bmatrix} \mathbf{O}_3 & \mathbf{O}_3 & c_2 k_1'' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & -k_1'' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ -k_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \\ \mathbf{O}_3 & -l_2' \mathbf{I}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 & \mathbf{O}_3 \end{bmatrix} \] (24)

Note that variables \( \chi' = \text{Re}(\chi) \) and \( \chi'' = \text{Im}(\chi) \). For simplicity, we have assumed single complex conjugate pole-residue pair for now. \( \mathbf{I}_r \) and \( \mathbf{O}_r \) represent identity and null matrices with dimension \( r \times r \). We have also included electric current sources \( s_{ex}, s_{ey} \) and \( s_{ez} \) in the formulation.

A quick glance at Eq. (16) shows that its right-hand-side (RHS) still involves matrix operators \( \mathbf{A} \) and \( \mathbf{B} \) which incur considerable arithmetic operations and memory indexing, especially when one is solving the implicit update equations. Efforts have been made to further reduce such overheads by means of a more efficient ADI-FDTD method in lossless media proposed in [16, 17]. Such efficient ADI algorithm is included within a family of fundamental implicit schemes, which feature similar fundamental updating structures that are in simplest forms with most efficient matrix-operator-free RHS. Following [17], it can be shown that Eq. (16) is reducible to the fundamental form (FADI-FDTD), which calls for the following update procedures:

\[ \tilde{\mathbf{v}}^n = [(\mathbf{I}_{12} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^n - \tilde{\mathbf{v}}^{n-\frac{1}{2}} \] (25a)

\[ (\mathbf{I}_{12} - \mathbf{D}_2 \mathbf{A} + \mathbf{F}_l) \mathbf{u}^{n+\frac{1}{2}} = \tilde{\mathbf{v}}^n + \mathbf{D}_2 \mathbf{s}^{n+\frac{1}{2}} \] (25b)

\[ \tilde{\mathbf{v}}^{n+\frac{1}{2}} = [(\mathbf{I}_{12} + \mathbf{D}_1) + \mathbf{F}_l + \mathbf{F}_r] \mathbf{u}^{n+\frac{1}{2}} - \tilde{\mathbf{v}}^n \] (25c)

\[ (\mathbf{I}_{12} - \mathbf{D}_2 \mathbf{B} + \mathbf{F}_l) \mathbf{u}^{n+1} = \tilde{\mathbf{v}}^{n+\frac{1}{2}} \] (25d)

where Eq. (25a) and Eq. (25b) form the first substep while Eq. (25c) and Eq. (25d) form the second. It is worth noting that the FADI-FDTD has matrix-operator-free RHS, i.e., there is no
matrix operator $A$ and $B$ on the RHS of Eq. (25). The source excitation is also only needed at the first substep [21] which further simplifies the implementation compared to the conventional ADI-FDTD method.

We now provide the full update equations of FADI-FDTD from Eq. (25). Letting

$$
\vec{v} = [e_x, e_y, e_z, h_x, h_y, h_z, \vec{j}_x, \vec{j}_y, \vec{j}_z, \vec{m}_x, \vec{m}_y, \vec{m}_z, \vec{m}_x', \vec{m}_y', \vec{m}_z', \vec{m}_x'', \vec{m}_y'', \vec{m}_z'']^T,
$$

we have for the first substep,

$$
v_x^n = (1 + c_2)E_{x}^{n-\frac{1}{2}} - c_2 \sum_p \text{Re} \left\{ (1 + k_{1p})J_{x|p}^{n} \right\}, \quad \xi = x, y, z
$$

$$
h_y^n = (1 + d_2)H_{y}^{n-\frac{1}{2}} - d_2 \sum_p \text{Re} \left\{ (1 + l_{1p})M_{y|p}^{n} \right\}, \quad \xi = x, y, z
$$

$$
j_{x|p}^{n-\frac{1}{2}} = (1 + k_{1p})p_{x|p}^{n} - \rho_{x|p}^{n-\frac{1}{2}} - 2k_{2p}E_{x|p}^{n}, \quad \forall p, \quad \xi = x, y, z
$$

$$
m_{x|p}^{n} = (1 + l_{1p})M_{x|p}^{n} - m_{x|p}^{n-\frac{1}{2}} - 2l_{2p}H_{x|p}^{n}, \quad \forall p, \quad \xi = x, y, z
$$

$$
E_{x}^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} H_{x}^{n+\frac{1}{2}} = e_x^n - c_2 s_{ex}
$$

$$
E_{y}^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial z} H_{y}^{n+\frac{1}{2}} = e_y^n - c_2 s_{ey}
$$

$$
E_{z}^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial x} H_{z}^{n+\frac{1}{2}} = e_z^n - c_2 s_{ez}
$$

$$
H_{x}^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial z} E_{x}^{n+\frac{1}{2}} = h_x^n
$$

$$
H_{y}^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial x} E_{y}^{n+\frac{1}{2}} = h_y^n
$$

$$
H_{z}^{n+\frac{1}{2}} - d_2 \frac{\partial}{\partial y} E_{z}^{n+\frac{1}{2}} = h_z^n
$$

$$
J_{x|p}^{n+\frac{1}{2}} = k_{2p}E_{x|p}^{n+\frac{1}{2}} + j_{x|p}^{n-\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z
$$

$$
M_{x|p}^{n+\frac{1}{2}} = l_{2p}H_{x|p}^{n+\frac{1}{2}} + m_{x|p}^{n-\frac{1}{2}}, \quad \forall p, \quad \xi = x, y, z.
$$

The second substep can be similarly written down by expanding Eq. (25c) and Eq. (25d). To solve for $E_x$ implicitly, Eq. (27j) is substituted into Eq. (27e) to yield

$$
E_{x}^{n+\frac{1}{2}} - c_2 \frac{\partial}{\partial y} (d_2 \frac{\partial}{\partial y} E_{x}^{n+\frac{1}{2}}) = e_x^n - c_2 s_{ex} + c_2 \frac{\partial}{\partial y} h_y^n.
$$

The advantages of the FADI-FDTD over the conventional ADI-FDTD can be summarized as follows:

1) Matrix-operator-free RHS in FADI-FDTD, c.f. Eq. (25). On the other hand, the RHS of conventional ADI-FDTD still involves matrix operators $A$ and $B$, c.f. Eq. (16).

2) Source excitation is only needed in first substep of FADI-FDTD, c.f. Eq. (25b), compared to both substeps of conventional ADI-FDTD, c.f. Eq. (16a) and Eq. (16b).

3) Implicit update equation of FADI-FDTD, c.f. Eq. (28) is much simpler compared to that of conventional ADI-FDTD, c.f. Eq. (15).
4) Implicit update equation of FADI-FDTD, c.f. Eq. (28) has much lesser spatial differential operators than that of conventional ADI-FDTD, c.f. Eq. (15). Thus, applying finite difference approximation to these spatial differential operators will incur less overheads in FADI-FDTD compared to conventional ADI-FDTD.

5) No dispersive terms $J$ and $M$ is required in implicit update equation of FADI-FDTD, c.f. Eq. (28). On the other hand, they are required in implicit update equation of conventional ADI-FDTD, c.f. Eq. (15).

6) The overall number of RHS terms in FADI-FDTD are lesser than that of conventional ADI-FDTD. This reduces the amount of arithmetic operations, memory indexing, and results in higher efficiency.

4. Numerical results

4.1. Transmission and reflection coefficients

To demonstrate the accuracy of our hemoglobin model in the FADI-FDTD method, we first compute the transmission and reflection coefficients of a half space human blood numerically. A modulated Gaussian pulse is launched from free space and upon hitting the human blood interface, undergoes transmission and reflection. The modulated Gaussian pulse has a bandwidth of 1500 THz around centre frequency of 750 THz, thus covering the entire frequency spectrum of the human blood model (300 THz to 1200 THz). The model of 15 g/dL hemoglobin concentration (Table 1) is used. Cell size is set at 3.125 nm which corresponds to cell per wavelength (CPW) of around 50 for the shortest wavelength in the human blood (wavelength in human blood, $\lambda \approx \lambda_0/1.5$, where $\lambda_0$ is the wavelength in free space. The shortest wavelength considered in free space is 250 nm). The time step $\Delta t$ is always specified as Courant-Friedrich-Lewy number (CFLN), which is relative to the Courant-Friedrich-Lewy time step limit in the explicit Yee’s FDTD method, i.e. $CFLN = \Delta t/\Delta t_{CFL}$ where $\Delta t_{CFL}$ is the maximum allowed time step of explicit FDTD method in Eq. (1).

The transmission and reflection coefficients (in frequency domain) can be obtained numerically by taking the ratio of the discrete Fourier transform of the transmitted and reflected wave, respectively to the discrete Fourier transform of the incident wave. The numerical experiment is run for various CFLNs to validate the accuracy of the hemoglobin model under different time steps. Figure 4 graphs the magnitude of the computed (a) transmission and (b) reflection coefficients, respectively versus frequency for various CFLNs. They are compared against the reference transmission and reflection coefficients of our analytical hemoglobin model. Also shown in the figures are the transmission and reflection coefficients computed using the explicit FDTD method. Since the explicit FDTD method is not unconditionally stable, it is run at its maximum time step limit of CFLN=1. Any time step larger than that will render the algorithm unstable. The FADI-FDTD method is unconditionally stable, and therefore we can see that CFLN beyond 1 still yield considerably accurate results. Nevertheless, the accuracy of the FADI-FDTD method deteriorates as the CFLN increases, especially towards higher frequency region. This is because as the frequency increases, higher CFLN (and thus larger time step) fails to resolve these higher frequency components sufficiently. Therefore, larger chosen time step increases the simulation speed, but at the expense of sacrificing a certain degree of accuracy. Based on these results, we can see that the chosen time step in FADI-FDTD is always a compromise between efficiency and accuracy.
4.2. Specific absorption rate (SAR)

The specific absorption rate (SAR) is an important measure for biological media exposed to electromagnetic radiation, which describes the electromagnetic energy absorption rate. It is defined as

\[ \text{SAR} = \frac{s_l}{\rho} \]  

(29)

where \( s_l \) is the power loss density in W/m\(^3\) and \( \rho \) is the density of the biological media in kg/m\(^3\), which gives the SAR the overall unit of W/kg. In most of the previous SAR analysis literatures [22–25], the power loss density is usually computed using

\[ s_l = \frac{1}{2} \sigma |\vec{E}|^2 \]  

(30)

where \( \vec{E} \) is the phasor form (without time dependence) of the electric field components. In time domain methods, such as the FDTD methods, the significant benefit is such that a narrow pulse can be injected to provide a wide range of frequency points using only a single run of simulation. In this case, \( \vec{E} \) can be the Fourier transform of the recorded electric field components, which gives us the information across a range of frequency resulted from illumination by any sinusoidal (monochromatic) source. This however, can only be performed if the medium of interest is modeled as the simplest case of conductive media, described by only a single conductivity value across the frequency range of interest. This is usually not the case in most biological media, such as the human blood described in this paper, where the conductivity changes with frequency. To use Eq. (30), the simulation has to be carried out point by point across the frequency range of interest using sinusoidal excitation, along with the corresponding conductivity values at different frequency. The advantage of FDTD method is thus not being exploited fully.

Since we have successfully modeled human blood across a range of optical frequency based on complex conjugate pole-residue pairs along with its implementation using the FADI-FDTD method, the power loss density formula in Eq. (30) can be modified to better suit our scenario. For a dispersive medium which has a complex permittivity of \( \varepsilon = \varepsilon' - j\varepsilon'' \), where \( \varepsilon' \) and \( \varepsilon'' \) are the real and negative imaginary (dissipative) parts, respectively, the power loss density can be...
Fig. 5. SAR (in logarithmic scale) at different locations of capillary at 440 THz (680 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

found using [26, 27]

\[ s_l = \frac{1}{2} \omega \varepsilon'' |\tilde{E}|^2. \]  

Equation (31)

Note that for conductive media with single conductivity value, \( \varepsilon'' = \sigma / \omega \) and Eq. (31) conforms to Eq. (30), which is considered as a special case for simplest conductive media. Hence, Eq. (31) is the generalization of power loss density for dispersive media. Using Eq. (31), we are now able to obtain the information across a range of frequency with only a single run of simulation, which is highly efficient.

In the following numerical example, we consider a capillary (blood vessel) in our body, and has a typical diameter of 8 \( \mu \)m. The straight long capillary is oriented along \( z \)-direction and is surrounded by tissue, which is assumed to be made up of mostly water and thus, having similar dielectric properties of water. Since the water has negligible absorption in the visible light and near infrared region, the refractive index is taken as a constant value of 1.33. Both models of 15 g/dL and 33 g/dL hemoglobin concentrations are applied to the capillary. The cell size is chosen as 11.1 nm which corresponds to CPW of 15 at shortest wavelength in the human blood and the time step is chosen at CFLN=4. A \( z \)-directed line current source of the same modulated Gaussian pulse as the previous subsection illuminates upon the capillary, exciting the frequency contents from 300 THz to 1200 THz. The perfectly matched layer [28] terminates the computational boundaries.

At steady state, the SAR values at different locations of the capillary are computed using Eq. (29) and Eq. (31) and the density, \( \rho \) of the human blood is 1060 kg/m\(^3\) [25]. The SAR is computed at frequencies of 440 THz, 550 THz and 720 THz. These frequencies correspond to free space wavelengths of 680 nm, 545 mm and 417 nm. Referring to Fig. 3, wavelength at 417 nm is where the highest absorption peak occurs, followed by 545 nm. The lowest absorption occurs at 680 nm. Figs. 5, 6 and 7 illustrate the SAR values (in W/kg) at different locations of the capillary at 440 THz, 550 THz and 720 THz, respectively. All the SAR values are plotted in logarithmic scale (\( \log_{10} \text{SAR} \)). All figures (a) refer to hemoglobin concentration of 15 g/dL while figures (b) refer to hemoglobin concentration of 33 g/dL. The SAR values at each location have been scaled to correspond to incident power density \( S = \frac{1}{2} \text{Re}(\tilde{E} \times \tilde{H}^*) \) of 1 mW/m\(^2\) in free
Fig. 6. SAR (in logarithmic scale) at different locations of capillary at 550 THz (545 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

Fig. 7. SAR (in logarithmic scale) at different locations of capillary at 720 THz (417 nm) for hemoglobin concentrations of (a) 15 g/dL and (b) 33 g/dL. The wave illuminates from left to right.

space. Note that the source illuminates from the left to right of the figures. We first notice that frequency at 720 THz (417 nm), c.f. Fig. 7 gives rise to the highest SAR values, followed by 550 THz (545 nm), c.f. Fig. 6 and 440 THz (680 nm), c.f. Fig. 5. This is in consistent with the absorption coefficient profile in Fig. 3. Another interesting observation is that at only 720 THz (417 nm), the SAR in the capillary shows a descending trend from the left to right along the wave travelling direction, while other frequencies show rather uniform SAR across the whole capillary region. This indicates that at the absorption peak of 720 THz (417 nm), the bulk of the power is absorbed near the left side, which results in lesser power penetration across the capillary. On the other hand, the absorbed power is well distributed across the whole region of the capillary at other frequencies due to weaker absorption. The standing wave effect may be attributed to the closed volume of the capillary. At the same time, it is observed that capillary
Table 3. Maximum and Average SAR Values Computed using FADI-FDTD and Explicit FDTD at Hemoglobin Concentration of 15 g/dL

| Frequency/Wavelength | FADI-FDTD | explicit FDTD |
|----------------------|-----------|---------------|
|                      | SAR max  | SAR avg       | SAR max  | SAR avg       |
|                      | (W/kg)   | (W/kg)        | (W/kg)   | (W/kg)        |
| 440 THz (680 nm)     | 2.4870 × 10^{-4} | 1.5662 × 10^{-4} | 2.5134 × 10^{-4} | 1.5659 × 10^{-4} |
| 550 THz (545 nm)     | 0.0438   | 0.0243        | 0.0445   | 0.0247        |
| 720 THz (417 nm)     | 0.2783   | 0.0969        | 0.2758   | 0.0964        |

Table 4. Maximum and Average SAR Values Computed Using FADI-FDTD and Explicit FDTD at Hemoglobin Concentration of 33 g/dL

| Frequency/Wavelength | FADI-FDTD | explicit FDTD |
|----------------------|-----------|---------------|
|                      | SAR max  | SAR avg       | SAR max  | SAR avg       |
|                      | (W/kg)   | (W/kg)        | (W/kg)   | (W/kg)        |
| 440 THz (680 nm)     | 0.0012   | 4.5712 × 10^{-4} | 0.0012   | 4.5704 × 10^{-4} |
| 550 THz (545 nm)     | 0.1574   | 0.0491        | 0.1654   | 0.0510        |
| 720 THz (417 nm)     | 0.6021   | 0.0914        | 0.5973   | 0.0906        |

with hemoglobin concentration of 33 g/dL generally exhibits higher SAR values across all frequencies. This concentration represents that of only the red blood cells, and could possibly model blood clot inside a capillary, which is formed as a result of entrapment of red blood cells [29]. Thus, the SAR calculation reveals that blood clot has a higher absorption compared to normal blood, which could be useful for medical applications and diagnostics.

We have also performed similar numerical example using the explicit FDTD method. Tables 3 and 4 show the maximum and average SAR of the capillary computed using the FADI-FDTD method and explicit FDTD method at hemoglobin concentrations of 15 g/dL and 33 g/dL. It can be seen that the calculated SAR values are quite close to each other. This shows that using the FADI-FDTD method at CFLN=4 does not suffer too much from accuracy deficiency. It is also found that the simulation time incurred by the FADI-FDTD method at CFLN=4 in Matlab codes is around 3 times faster than that of the explicit FDTD method. These further show that while maintaining accuracy, the FADI-FDTD method is promising in achieving higher efficiency for modeling biological media.

5. Conclusion

This paper has presented the modeling of hemoglobin at optical frequency (250 nm - 1000 nm) using the unconditionally stable fundamental alternating-direction-implicit finite-difference time-domain (FADI-FDTD) method. An accurate model based on complex conjugate pole-residue pairs has been proposed to model the complex permittivity of hemoglobin at optical frequency. Two hemoglobin concentrations at 15 g/dL and 33 g/dL have been considered. The model is then incorporated into the FADI-FDTD method for solving electromagnetic problems involving interaction of light with hemoglobin. The computation of transmission and reflection coefficients of a half space hemoglobin medium using the FADI-FDTD has validated the accuracy of our model and method. The specific absorption rate (SAR) distribution of human capillary at optical frequency has also been shown. While maintaining accuracy, the unconditionally stable FADI-FDTD method has exhibited high efficiency in modeling hemoglobin.