Comparison of different formulations for transient radiative transfer problems in absorbing and scattering three-dimensional media

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ABSTRACT: Four different formulations for the solution of transient radiative transfer in a three-dimensional absorbing and scattering medium are compared in this work. Two of these formulations are frequently used and well-known in the radiative transfer community: the radiative transfer equation, and the diffusion equation, based on the P1 approximation. The other two are based on a multi-scale approach, where the radiative intensity is decomposed into a macroscopic and a mesoscopic components. One of these multi-scale models is called the hybrid transport-diffusion model, while the other is called the micro-macro model. The major difference between the two multi-scale models lies in the way the macroscopic component is defined. These multi-scale models aim to improve the efficiency of the numerical simulation of radiative transfer in transient problems. This kind of problems appears, for example, in optical tomography applications, where the propagation of a laser inside a biological tissue must be simulated efficiently in order to determine the optical properties of the tissue and to detect the presence of tumours or inhomogeneities. In this thesis the various formulations are compared for an academic configuration consisting of a cubic absorbing and scattering medium subject to collimated radiation. The influence of both the discretization schemes (spatial and temporal) and the optical parameters is also investigated. The results show that second-order accurate discretization schemes greatly improve the solution accuracy when the optical thickness of the medium and the scattering albedo are large. The two multi-scale models improve the accuracy of the results, especially with the first-order discretization schemes, and the computational efficiency of the calculations when the scattering optical thickness is large.

KEY-WORDS: Radiative transfer; Discrete ordinates method; P1 approximation; Diffusion approximation; Hybrid transport-diffusion model; Micro-macro model.

1 INTRODUCTION

As widely known, the interest in the study of transient radiative transfer has been increasing for the last few decades. Many research fields, such as optical tomography, laser micromachining, remote sensing and others make use of short pulse lasers that require to take into account transient effects [1].

Various models have been developed and tested over the years to solve the transient radiative transfer equation (RTE) [2] with different results and trade-offs, such as the Monte Carlo (MC), the finite volume method (FVM) and the discrete ordinates method (DOM). Although the RTE is extensively used, the approximate diffusion equation (DE) is sometimes preferred, particularly in optically thick media, due to the lower computational requirements.

In the present work, four three-dimensional radiative transfer formulations are compared: the RTE, the DE, the hybrid transport-diffusion model (HTD) [3] and the micro-macro model (MM) [4]. The last two formulations
are multi-scale models developed in our previous works. In the RTE, the radiation intensity is decomposed into a collimated component, associated to the laser beam incident on the domain under consideration, and a diffuse component. Hence, the RTE yields two transport equations, each one for a component of the radiation intensity. This is the first formulation considered in the present work. The second one is a simplified formulation obtained when the P1 and the diffusion approximations for the diffusive component are used, yielding the so-called diffusion equation. The two multi-scale models tested in this study are based on the decomposition of the diffuse component of the radiation intensity into a macroscopic component and a mesoscopic one. The major difference between the two multi-scale models lies in the way the macroscopic component is defined. In the HTD model, the macroscopic component is chosen equal to the solution of the diffusion equation, while in the MM model the macroscopic component is defined as the incident radiation (the integral of the radiative intensity over the solid-angle space).

In the present work, the efficiency of the various models, regarding accuracy and computational requirements (CPU time), are compared for a three-dimensional test case related to optical tomography applications, following previous one-dimensional applications reported in [3-4].

2 THEORY

2.1 Radiative transfer models

2.1.1 Radiative Transfer Equation

The transient radiative transfer equation (RTE) for absorbing and scattering media can be written as [2]:

$$\frac{1}{c} \frac{\partial I}{\partial t} + u \cdot \nabla I = -(k_a + k_s)I + k_s \int_{4\pi} p(u \cdot u') I' \, d\Omega'$$  \hspace{1cm} (1)

where $I = I(x,u,t)$ represents the radiation intensity at location $x$, propagation direction $u$ and time $t$. The speed of light is represented by $c$, $k_a$ is the absorption coefficient, $k_s$ is the scattering coefficient, $p$ is the normalized scattering phase function, $u'$ is the incident direction and $I'$ stands for $I(x,u',t)$. When the medium is subjected to laser irradiance it is convenient to decompose the radiation intensity into its collimated component, $I_c$, and its diffuse component, $I_d$, according to $I(x,u,t) = I_c(x,u,t) + I_d(x,u,t)$. Thus, two equations are obtained:

$$\frac{1}{c} \frac{\partial I_c}{\partial t} + u \cdot \nabla I_c = -(k_a + k_s)I_c$$  \hspace{1cm} (2)

$$\frac{1}{c} \frac{\partial I_d}{\partial t} + u \cdot \nabla I_d = -(k_a + k_s)I_d + k_s \int_{4\pi} p(u \cdot u') I'_d \, d\Omega' + k_s p(u \cdot u_c)I_c$$  \hspace{1cm} (3)

Subscripts $c$ and $d$ stand for the collimated and diffusive components, respectively.

2.1.2 Diffusion Equation

The diffusion equation (DE) can be deduced by integrating the RTE over a solid angle and applying the $P_1$ approximation expressed by $I_d(x,u,t) \approx I_d^{\text{lim}}(x,u,t) = \left[ G_d \, \text{lim} (x,t) + 3 u \cdot u_d \right] / 4\pi$, where $G$ is the incident radiation, $q$ the radiative heat flux vector, and superscript $\text{lim}$ denotes the diffusion limit. The following DE is obtained for the diffuse component:
\[
\frac{1}{c} \frac{\partial G_{d}^{\lim}}{\partial t} - \nabla \cdot \left( D \nabla G_{d}^{\lim} \right) = -k_a G_{d}^{\lim} + k_s I_{c} - \nabla \cdot \left( 3 D k_s g I_{c} u_{c} \right) \tag{4}
\]

where \( D \) is the diffusion coefficient, given by \( D = \left[ k_a + k_s \left( 1 - g \right) \right] / 3 \), and \( g \) is the asymmetry factor of the phase function [2].

2.1.3 Micro-Macro model

In the MM model the diffuse component is decomposed as \( I_{d}(x, u, t) = G_{d}(x, t)/4\pi + \varepsilon_{d}(x, u, t) \). The incident radiation, \( G_{d} \), is the macroscopic component, and it can be shown that it satisfies the following equation:

\[
\frac{1}{c} \frac{\partial G_{d}}{\partial t} + \langle u \cdot \nabla \varepsilon_{d} \rangle = -k_a G_{d} + k_s I_{c} \tag{5}
\]

where symbol \( \langle \cdot \rangle \) represents the integral over the solid-angle space of \( 4\pi \). The transport equation for the mesoscopic component, which results from the RTE, is the following [4]:

\[
\frac{1}{c} \frac{\partial \varepsilon_{d}}{\partial t} + u \cdot \nabla \varepsilon_{d} = -(k_a + k_s) \varepsilon_{d} + k_s \int_{4\pi} p(u \cdot u') \varepsilon_{d}' du' + k_s I_{c} \left[ p(u \cdot u_{c}) - \frac{1}{4\pi} \right] + \frac{1}{4\pi} \left( \langle u \cdot \nabla \varepsilon \rangle + u \cdot \nabla G \right) \tag{6}
\]

The system of equations (2), (5) and (6) is equivalent to the transient RTE. However, the exact boundary conditions are not preserved. In this case, artificial boundary conditions of Neumann type are used (see [4] for details).

2.1.4 Hybrid Transport-Diffusion model

The HTD model relies on a diffuse component decomposition similar to that used in the MM model, according to \( I_{d}(x, u, t) = G_{d}^{\lim}(x, t)/4\pi + \varepsilon_{d}(x, u, t) \). The difference is that the macroscopic unknown in the HTD model is the incident radiation at the diffusive limit, \( G_{d}^{\lim} \), which satisfies the diffusion equation (DE). The transport equation for the mesoscopic component, \( \varepsilon_{d} \), is deduced from Eqs. (3) and (4) yielding:

\[
\frac{1}{c} \frac{\partial \varepsilon_{d}}{\partial t} + u \cdot \nabla \varepsilon_{d} = -(k_a + k_s) \varepsilon_{d} + k_s \int_{4\pi} p(u \cdot u') \varepsilon_{d}' du' + k_s I_{c} \left[ p(u \cdot u_{c}) - \frac{1}{4\pi} \right] + \frac{1}{4\pi} \left[ \nabla \cdot \left( 3 D k_s g I_{c} u_{c} - D \nabla G_{d}^{\lim} \right) - u \cdot \nabla G_{d}^{\lim} \right] \tag{7}
\]

Unlike the MM model, the three governing equations (2, 4 and 7) are decoupled, which means that the equations for the HTD model are simpler to solve than those for the MM model.

The exact boundary conditions for the radiation intensity are conserved in the HTD model. The boundary conditions for \( \varepsilon_{d} \) are defined according to that chosen for \( G_{d}^{\lim} \), in order to match the exact radiation intensity on the walls. The Marshak boundary conditions were used for \( G_{d}^{\lim}(x_w, t) \) [2].

2.2 Numerical Schemes

Analytical solutions to the radiative transfer equation (RTE) exist for simple cases but numerical methods are required for more realistic media with complex multiple scattering effects. When numerical methods are used, the continuous domain of the problem is approximated by a discretized one using discretization schemes.
The RTE for the diffuse component, Eq. (3), and Eqs. (6) and (7) of the multi-scale models were solved using the discrete ordinates method (DOM). In the DOM, the governing integro-differential equation is replaced by a discrete set of $N$ coupled equations that describe the radiation intensity (or mesoscopic component) field along $N$ directions. A quadrature replaces the integrals over solid angles. In this study, an $S_{12}$ quadrature was employed. The spatial discretization was carried out using the finite volume method. The convective-like term was discretized using either the step scheme (first-order accurate) or the CLAM scheme (second-order accurate). The transient term was also discretized using either a first order (explicit Euler) or a second-order (Runge-Kutta) scheme. Depending on the radiative properties of the problem under consideration, the discretization schemes may be critical in order to achieve accurate results once, as is largely known, they are largely susceptible to several error generating phenomena: ray effect, numerical diffusion and false radiation [5]. This shown in the results presented below.

3 TEST CASE

A simple three-dimensional test case was considered to compare the accuracy and efficiency of the different models and discretization schemes. It consists of a three-dimensional cubic enclosure of side $L=1\,\text{m}$, schematically shown in Fig. 1, containing a scattering and absorbing homogeneous medium and subjected to an incident laser source in one boundary, while the remaining boundaries are black (absorb all incident radiation) and cold (non-emitting). The medium is cold, as often considered in problems of light propagation in biological tissues, and the scattering is described by the Henyey-Greenstein phase function [2]. A pulse laser Gaussian in time and uniform in space is simulated according to:

$$I_c(x_o, u, t) = I_o \, \delta(u - u_c) \exp\left[-4 \left(\ln 2\right)\left(t - t_c\right)/(t_p)^2\right], \quad 0 < t < 2t_c$$  \hspace{1cm} (8)

where $x_o$ is the emitting wall location, $\delta$ is the Dirac delta function and $I_o$ is the maximum radiative intensity of the pulse, which occurs at $t = t_c = 3t_p$. A dimensionless time parameter defined as $t_p^* = c \left(k_a + k_s\right) t_p$ is fixed equal to 0.5. The laser is normal to the boundary (see Fig. 1). After $2t_c$ the medium is free from irradiation. In this work we are concerned with the temporal signature of the incident radiation at the wall opposite to the laser. This is quantified by the dimensionless transmittance given by:

$$T(t) = T_c(t) + T_d(t) = \frac{I_c(x_L, u, t)}{I_o} u \cdot n + \int_{2\pi} \frac{I_d(x_L, u, t)}{I_o} (u \cdot n) du$$  \hspace{1cm} (9)

where $x_L$ is the wall located at $(x=L, y, z)$ and $n$ is the unit vector normal to the wall in positive $x$ direction.

A simulation is defined by three main optical parameters: optical thickness, $\tau = (k_a+k_s)\times L$, albedo, $\omega_a$ and

![Figure 1- Schematic of the test case.](image)
asymmetry factor, \( g \). The influence of each individual parameter on the transmittance is investigated. A previously validated Monte Carlo algorithm [3] is used to provide benchmark results.

4 RESULTS

The enclosure is divided into 50 divisions in the \( x \) direction \((N_x=50)\) and 20 divisions in both \( y \) and \( z \) directions \((N_y=N_z=20)\), resulting in \( \Delta x=0.02 \text{ m} \) and \( \Delta y=\Delta z=0.05 \text{ m} \). This finer mesh along the \( x \) direction provides a better trade-off between accuracy and computational effort than a mesh equally refined in all directions, once it is refined just in the collimated direction. The time step \( \Delta t \) is defined as \( \Delta t=\alpha.\Delta x/c \), for the RTE, HTD and MM formulations, and as \( \Delta t=\alpha.\Delta x^2/(10D.c) \) for the DE, where the stability parameter \( \alpha \) was set equal to 0.5.

An isotropic basis scenario is set in Fig. 2, with \( \tau=10, \omega=0.5 \) and \( g=0 \). The 1st order spatial and temporal schemes in Fig. 2(a) already show a close agreement with the MC prediction. In these conditions the DE model proves to be the most accurate while the RTE presents the biggest errors, both in the peak and steep rise regions of the curve, which according to its shape is essentially transmitted collimated radiation. The multi-scale models provide better results comparatively to RTE, in both aspects. Increasing the order of the temporal scheme from a 1st order Euler to a 2nd order Runge-Kutta (RK2) scheme has a positive localised effect on the peak value of the models, as visible in Fig. 2(b). However this positive impact is negligible for DE where the results improved less than 1%, probably due to the fact that \( \Delta t \) for this model is already so small that a higher order scheme in time has no tangible effect. Meanwhile, using only a 2nd order scheme in space (CLAM scheme), Fig. 2(c), also provides a localised accuracy increase, but now in the abrupt rise region of the curve, basically attenuating the numerical diffusion and false radiation phenomena, as verified in previous studies. The errors caused by numerical diffusion

![Fig 2](image.png)

**Figure 2** - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for \( \tau=10, \omega=0.5, g=0 \).
and false radiation lead to solutions with unphysical radiation since the transmittance becomes different from zero well before the first collimated photons reach the boundary at \( x = L \) and \( t = L/c = 3.33 \times 10^{-9} \) s. Finally, in Fig. 2(d), the 2nd order spatial and temporal schemes are combined, providing better results than the simple sum of its individual parts, i.e., the overall impact is greater than the sum of the localised positive effects discussed in Figs. 2(b) and (c). Despite the results of RTE, MM and HTD in Fig. 2(d) being slightly more precise than DE, this last model requires a lower CPU time by several orders of magnitude, being more attractive for the present case.

In the case of anisotropic scattering, the asymmetry factor is no longer zero. In Fig. 3, \( g = 0.3 \) while the remaining optical parameters are kept constant. The first thing to notice by comparing Figs. 2(a) and 3(a), apart from the nearly 35% rise in the magnitude of the peak, is the increased difficulty of the 1st order schemes to precisely describe the transmittance signal. For different reasons, the various models fail to represent closely the asymmetry of the MC curve. This asymmetry is a consequence of the diffuse component growth, caused by the forward-peaked scattering that extends the signal after the collimated peak. While the mesoscopic/multi-scale models cannot capture the sudden rise of the curve, due to the usual error phenomena, the DE model, which performed fairly well in the isotropic case, exhibits considerable peak and post-peak errors, i.e., it underestimates the diffuse component. Fig. 3(b) shows that the RK2 as no impact in the accuracy of the DE model but provides a minor localised (peak) improvement for the RTE, MM and HTD. However the major improvement comes from the CLAM scheme (Fig. 3(c)), cancelling much of the false radiation. Of course, associating both spatial and temporal 2nd order methods leads to the best results, with the overlapping of the tested models, but does not completely eliminate the numerical errors. The CPU times for case (d) are (from now on, when nothing is said, the CPU times always refer to the case of 2nd order spatial and temporal discretization schemes, since it is the most accurate): \( t_{MM} \approx 0.99 t_{RTE} \) and \( t_{HTD} \approx 1.04 t_{RTE} \).

![Figure 3 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for \( \tau = 10, \ \omega = 0.5, \ g = 0.3 \).](image-url)
When the optical thickness is raised to 20, maintaining $\omega$ and $g$ constant, the differences between the models and the various discretization schemes, and the false radiation and numerical diffusion errors, are magnified. The 1st order spatial and temporal schemes in Fig. 4(a) originate very large numerical errors for all the formulations, taking the Monte Carlo solution as reference. Physically, this optical thickness increase leads to increased absorption of radiation in the medium and therefore, in this specific case, the maximum transmittance decreases more than 4th orders of magnitude. Also, as the diffuse component of radiation contributes more to the overall transmittance, its temporal signature acquires an asymmetric nature that the macroscopic DE model is unable to simulate. For the remaining models, the error in the prediction of the maximum transmittance is of the order of magnitude of the collimated peak itself, resulting in a transmittance curve that has two peaks. In order to diminish the large error due to false radiation, and numerical diffusion, the RK2 and CLAM schemes are employed. Again, the RK2 as a low impact on the results (Fig. 4(b)) while the CLAM scheme largely reduces false radiation (Fig. 4(c)), but the errors remain large. Coupling the two 2nd order schemes is imperative to obtain the most accurate results, as represented in Fig. 4(d). However, in this scenario, they are not enough to achieve good results, and the errors introduced by false radiation, numerical diffusion and, may be, ray effect lead to a peak overestimation, of the order of 25%. There are several possible ways to reduce these errors, e.g. refine the spatial mesh, decrease the time step, employ different quadratures, apply even higher order discretization schemes, among others. The CPU times are $t_{\text{MM}} \approx t_{\text{RTE}}$ and $t_{\text{HTD}} \approx 1.02 t_{\text{RTE}}$. It is noted that the better performance of the multi-scale models, relatively to the RTE, is diluted with the higher order schemes and since higher order schemes are mandatory in the present case to obtain acceptable results and the CPU times are similar, there seems to be no advantage of the multi-scale models in comparison with the RTE.

Now the albedo is increased to 0.9 and its effect is displayed in Fig. 5. The temporal transmittance signature becomes longer, stronger, smoother and the maximum is achieved later than for $\omega = 0.5$, because the average residence time of the photons in the medium is higher due to the increased scattering coefficient. The transmittance

![Figure 4](image_url)

Figure 4 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=20$, $\omega=0.5$, $g=0.3$. 
profile is now virtually completely diffuse, once the collimated component is several orders of magnitude lower than the diffuse one. Both multi-scale models out-perform consistently the RTE model with the lower order schemes. It is emphasized that, unlike in the previous scenario (Fig. 4), the errors with the 2nd order spatial and temporal schemes are no longer significant and the multi-scale models are an alternative to consider (e.g. Fig. 5(c)). This is due to the fact that the transmittance is now smoother and more symmetrical, as opposed to the previous case, which is more favourable to the macroscopic component of the multi-scale models. The CPU relations are \( t_{MM} \approx t_{RTE} \) and \( t_{HTD} \approx 1.03 t_{RTE} \). The MC oscillations could be overcome by increasing the number of photon bundles.

Additionally, to further complement the anisotropic investigation, the forward-peaked scattering is intensified by setting the asymmetry factor to \( g = 0.6 \). The scenario \( \tau = 20, \omega = 0.9, g = 0.6 \) is displayed in Fig. 6. The increase of the asymmetry factor yields a narrower transmittance signal, the peak occurs earlier and its value rises. With twice the asymmetry factor, the maximum transmittance increases about tenfold. As we move away from the isotropic conditions, the shape of the DE’s curve is increasingly departing from the one predicted by the MC model. Despite the underestimation of the post-peak transmittance, the multi-scale HTD model, along with the MM, performs better than the RTE for the several schemes in Figs. 6 (a), (b) and (c). However, the combination of the CLAM and RK2 schemes does not solve this underestimation problem and the HTD is then outperformed by the RTE, which takes more advantage from the higher order schemes (Fig. 6(d)). The relation between the CPU times is now \( t_{MM} \approx 1.01 t_{RTE} \) and \( t_{HTD} \approx 1.04 t_{RTE} \).

Figure 5 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for \( \tau=20, \omega=0.9, g=0.3 \).
Finally, a strong forward-peaked scattering case is studied. This highly demanding scenario ($\tau = 20, \omega = 0.9$ and $g = 0.9$) is designed to highlight and magnify the differences between the different formulations and schemes. First order schemes yield rather poor results for this scenario, and so only the 2nd order schemes are employed. In Fig. 7, the standard directional $50 \times 20 \times 20$ mesh (dashed line) is successively refined using a $100 \times 40 \times 40$ (dash-point lines) and a $200 \times 50 \times 50$ mesh (solid lines). It is stressed that the finer meshes are restricted to these two models for computational reasons, as the HTD model requires excessive memory allocation (the DE is no longer discussed and its results with the standard mesh are kept in the graphics just to give an idea of the error associated with it).

It becomes clear from Fig. 7 that the standard mesh is insufficient to accurately estimate the transmittance, which shows an hundredfold increase relatively to $g = 0.6$. Plenty unphysical radiation and an underestimation of the peak (and the curve in general) is observed. The three models behave similarly and the errors are transverse to all as far as $T(t)$ is concerned. This suggests that there is nothing wrong with the models themselves, but the discretization parameters are not satisfactory. The CPU times with the standard mesh are now $t_{MM} \approx 0.88 t_{RTE}$ and $t_{HTD} \approx 0.92 t_{RTE}$. This suggests that as the scenario becomes more demanding, the CPU effort of the multi-scale models decreases, relatively to the RTE model. As the meshes get more refined, the improvement is clear. The unphysical radiation, caused by false radiation and false scattering, practically disappears and the initial steep transmittance rise is captured precisely. However, a small peak underestimation error remains. This might be due to an inevitable residual ray effect associated with the DOM. Once more, the CPU time is favourable to the MM model with $t_{MM} \approx 0.90 t_{RTE}$ for $100 \times 40 \times 40$ and $t_{MM} \approx 0.91 t_{RTE}$ for $200 \times 50 \times 50$.

Figure 6 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=20$, $\omega=0.9$, $g=0.6$. 
5 CONCLUSION

Four different formulations for transient radiative transfer are compared, in three-dimensional absorbing and scattering media. The performance of these formulations is investigated using either first or second-order spatial and temporal discretization schemes and by changing the radiative properties of the medium. The effect of the numerical schemes on the accuracy of the models is very important if the optical thickness of the medium and the albedo are large, and the scattering is anisotropic. In such a case, increasing the order of accuracy of the spatial discretization scheme has a greater impact on the accuracy than increasing the order of accuracy of the temporal discretization, but using second order schemes for both spatial and temporal discretization yields the most accurate results. Still, in more demanding scenarios, numerical diffusion and false radiation may generate significant errors. However, the spatial mesh investigation shows that these phenomena are strongly reduced with smaller control volumes.

Overall, the results show that the multi-scale models perform either similarly or better than the other models and may be computationally more efficient than the RTE model, depending on the radiative properties of the medium. The DE model confirmed its limitations near the boundaries, where transmittance is defined, that are more obvious in more demanding scenarios.

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