Computational hybrid models for photon migration in biological tissues

MARINE KERVELLA
ISAIP-ESAIP Group
18 rue du 8 mai 1945, BP80022
49180 ST BARTHELEMY D'ANJOU
FRANCE

TANJA TARVAINEN
Department of Physics
University of Kuopio
P.O. Box 1627, FIN-70211 Kuopio
FINLAND

ANNE HUMEAU
ISAIP-ESAIP Group
18 rue du 8 mai 1945, BP80022
49180 ST BARTHELEMY D'ANJOU
FRANCE

JEAN-PIERRE L'HUILLIER
ENSAM, LPMI
2 boulevard du Ronceray, BP 3525
49035 Angers cedex
FRANCE

Abstract: In this paper, two numerical hybrid methods to model photon transport phenomena in biological tissues are compared. The coupled radiative transfer – diffusion model is based on the finite element solution of the radiative transfer equation and its approximation. The hybrid Monte Carlo – diffusion consists in modeling the propagation of laser light in turbid media with the pure statistical Monte Carlo method in the vicinity of the source and the boundaries and the diffusion approximation elsewhere in the domain. We apply these codes to calculate the spatially resolved reflectance amplitude and phase resulting from an intensity modulated laser beam. The results show that the hybrid methods can be used to simulate light propagation with good accuracy and speed.

Key–Words: Photon migration, Biomedical tissues, Finite element method, Monte Carlo, Radiative transfer equation, Diffusion approximation

1 Introduction

Near infrared spectroscopy has become a widely accepted method for investigating the human tissues structure. Laser light interaction with biological tissues is a complex process due to the multiple layers constituted by various cell types, each having different optical properties. Given the inhomogeneous nature of tissues it is important to develop adequate models to determine the nature of light information. Besides, it is essential for a number of optical diagnostic practices such as cancer detection at early stage, diabetes diagnosis and transplant inspection. A forward model for the propagation of light through tissues is needed in solving the inverse problem in optical imaging studies, but also for determining irradiation doses in photodynamic therapy treatments. Knowledge of the distribution of photon paths is the key to deciphering detected optical signals emerging from the surface of tissue. Therefore, propagation and distribution of light produced by illumination of turbid tissues have to be fast and efficiently estimated.

In this paper, we compare two computational hybrid models. The first numerical simulation of photon migration is based on the finite element method (FEM) under the consideration of the radiative transfer equation in the vicinity of the laser source and the diffusion approximation is used elsewhere in the domain [1,2]. The second one is based on a statistical numerical simulation, called Monte Carlo method, near the interfaces and the source areas and the diffusion approximation is used elsewhere. The light propagation models are described in Section 2. The hybrid method are tested with simulations in Section 3.

2 Methods

2.1 Light propagation models

The Radiative Transfer Equation

In optical tomography, the radiative transfer equation (RTE), referring forward to equation (1), is widely accepted as an accurate model for the propagation of light in biological tissues [3]. Based on the Boltzmann's equation, it considers the light propagation as the equivalent to the flow of discrete photons which may locally be absorbed or scattered by the medium. In the frequency domain, for monochromatic light, with $\Omega \subset \Re^3$ the physical domain, the RTE is of the form [3] :

$$\left(\frac{i\omega}{c} + \hat{s} \cdot \nabla + \mu_s + \mu_a\right) \phi\left(r, \omega, \hat{s}\right) =$$
$$\mu_s \int_{4\pi} \phi\left(r, \omega, \hat{s}'\right) \Theta\left(\hat{s} \cdot \hat{s}'\right) d\hat{s}' + q\left(r, \omega, \hat{s}\right) \qquad (1)$$

where $\phi\left(r, \omega, \hat{s}\right)$ is the energy radiance, μ_a and μ_s are the absorption and scattering coefficients of the medium, respectively, c is the speed of the light, ω is the angular modulation frequency of the input signal, $\hat{s}$ is unit vector in the direction of interest and $q(r, \omega, \hat{s})$ is the source term within the medium. The phase function $\Theta\left(\hat{s} \cdot \hat{s}'\right)$ describes the probability that a photon with an initial direction $\hat{s}'$ has the direction $\hat{s}$ after the scattering event. The RTE is computationally very expensive, and therefore it has been used as the forward model only in few applications.

The Diffusion Approximation

The most typical approach has been to replace the RTE by the diffusion approximation (DA). It is basically the first order approximation of equation (1) with respect to angular dependence [3,4]. In the frequency domain, the DA assumes the form

$$-\nabla \cdot \kappa \nabla \Phi(r, \omega) + \mu_a \Phi(r, \omega) +$$
$$\frac{i\omega}{c} \Phi(r, \omega) = q_0(r, \omega) \qquad (2)$$

where $\kappa = (3(\mu_a + \mu_s'))^{-1}$, is the diffusion coefficient, $\mu_s' = (1 - g)\mu_s$ is the reduced scattering coefficient, $g = \int_\theta \hat{s} \cdot \hat{s}' \Theta\left(\hat{s} \cdot \hat{s}'\right) d\hat{s}'$ is the mean cosine of the scattering angle and $\Phi(r, \omega) = \int_\theta \phi(r, \omega, \hat{s}) d\hat{s}$ is the photon density. The DA is a relatively good approximation to the RTE when the medium is scattering dominated, which is the case in most applications of optical tomography, and when the point of interest is not very close to the highly collimated light source and to boundaries.

The Coupled RTE-DA model

In the coupled RTE–DA model, see Fig.1, light propagation is modeled with the RTE in the sub-domain Ω_{rte} in which the approximations of the DA are not valid such as close to the source and domain boundary and within low-scattering and non-scattering regions [1,2]. The DA is used as the forward model in sub-domain Ω_{da} which is the remaining domain. The RTE and the DA are coupled on the interface Γ between the sub-domains using their boundary conditions. The coupled RTE–DA model can be solved with the FEM and it has been found to describe light propagation accurately in various media [1,2].

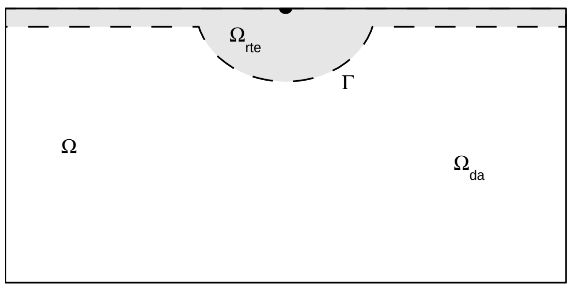

Figure 1: The domain Ω with the source at the centre of the upper edge. The RTE is used as the forward model in the sub-domain Ω_{rte} (grey colour); the DA is used as the forward model in the sub-domain Ω_{da}; the interface Γ separates the RTE and DA sub-domains (dashed line).

2.2 A hybrid Monte Carlo model

Classical Monte Carlo method

The classical Monte Carlo (MC) method is another numerical approach to simulate the photon migration in turbid tissues. It is often used to avoid DA failures. The principle of Monte Carlo simulation is based on probability functions of random numbers which describe the variable step size a photon will take between photon-tissue interaction sites, and the angle of deflection a scattered photon may experience due to a scattering event [5-7]. The aim of the MC method is to replace a deterministic problem by an equivalent stochastic problem. Therefore, its strategy is based on the random history of particles that is simulated.

The tissues are illuminated by a pencil photon beam which is normally incident. The trajectory of each photon packet in the media is studied until it reaches the detector. Once the photon packet has been moved, it is ready to be scattered. There will be a deflection angle, $\theta \in [0, \pi]$, and an azimuthal angle, $\Psi \in [0, 2\pi]$ to be sampled statistically. The probability distribution for the cosine of the deflection angle, $cos\theta$, is described by the scattering function that Henyey and Greenstein introduced [8]:

$$p(cos\theta) = \frac{1 - g^2}{2(1 + g^2 - 2gcos\theta)^{3/2}} \qquad (3)$$

where the parameter, g, equals $< \ cos\theta \ >$ and has a value between -1 and 1. A value of 0 indicates uniform scattering and a value near 1 indicates very forward directed scattering.

When the photon packet escapes from the domain, the quantities of interest are tallied and the results averaged over many particles histories.
MC method allows the direct handling of complex tissue geometries and optical inhomogeneities. So, it can be used to predict the light propagation in either a layered structure of extremities or a head model including a non scattering region [9]. Unfortunately, despite its reliability and because of its statistic aspects, the accuracy of scored quantities increases only with the square root of the number of photon histories and the method is computationally expensive.

Hybrid MC-DA method
Another numerical approach to overcome the limitations of diffusion is to develop a MC diffusion hybrid model that combines the accuracy of MC at short distances with the computational efficiency of diffusion at larger ones. Wang and Jacques [10] were the first to propose such a model for spatially resolved reflectance. Alexandrakis *et al.* [11], then, proposed solutions for frequency domain. In our study, the hybrid MC-DA method is developed and results are compared with previously described models.
The basic idea is to consider that the laser beam may be converted into deep isotropic sources when light reaches the middle zone of the biological media. This region is limited by two critical planes defined at respective depths $z_c = mfp$, with mpf the mean free path of photons before interaction with the medium, and $d - z_c$ where d is the depth of the medium (Fig. 2). Outside the central zone, the DA is inefficient. So, the propagation of photons packets is simulated by the classical MC method until they reach the middle zone. MC step allows to save the reflectance R_{mc} and the absorption matrix of photons which reached a position in the center zone. At the end of MC step, the absorption matrix terms are converted by the diffusion step. This process converts the infinitely narrow photon beam into a distributed source term and computes the additional diffuse reflectance R_{diff}. The latter is obtained in a manner similar to that described by Alexandrakis *et al.* in [11]. Our program proposes an optimized version in standard C, using approximated Gauss-Laguerre integrations in order to calculate rapidly the analytical solution R_{diff}, described by Kienle in [12]. Then, the final diffuse reflectance will be the sum of the diffuse reflectances computed by our two steps:

$$R(r,\omega) = R_{MC}(r,\omega) + R_{diff}(r,\omega)$$

3 Results and Discussion

In this section, we give numerical results in 2D cases. The solution of the forward problem was computed with the hybrid approaches on a 2.8 GHz PC with 2 Go RAM. We show results for two geometries, a slab and a two-layered domain and compare them with pure MC simulations. Both pure MC and hybrid MC model were implemented in C programming language. One million photon packets were traced in both models.
The coupled RTE–DA model was solved with the finite element method with the MATLAB version 7.0 (R14), (The MathWorks, Inc.). The RTE sub-domain included the regions close to the source and the upper boundary in which the measurements were performed (see Fig.1). The DA sub-domain included the remaining medium. The interface Γ located at the distance

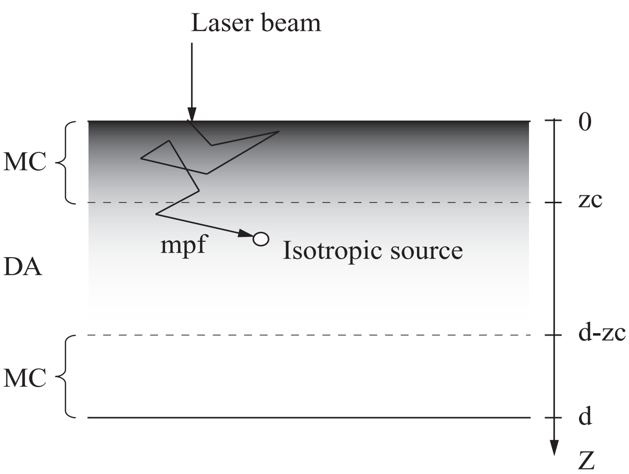

Figure 2: Illustration of the hybrid MC model.

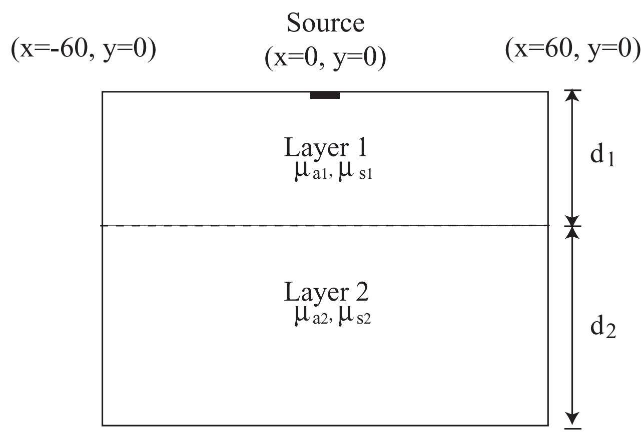

Figure 3: Schematic diagram of the physical domain.

Table 1: Optical coefficients for slab cases, $d_1 = 40$ mm and $d_2 = 0$ mm.

	$\mu_a\ (mm^{-1})$	$\mu'_s\ (mm^{-1})$
Slab 1	0.0015	0.1
Slab 2	0.0015	0.6
Slab 3	0.0015	1.2

of $2\,\mathrm{mm}$ from the upper boundary and $20\,\mathrm{mm}$ from the source. The FE-discretization of the slab contained 3428 triangular elements and the FE-discretization of the two-layer medium contained 4456 triangular elements.

The first simulations were carried out with a 40 mm x 60 mm rectangular slab (Fig.3 and Tab.1). The collimated light source was located at the center of the upper edge. The absorption coefficient of the medium is $\mu_a = 0.0015$ mm^{-1} and the scattering coefficient, μ_s, varies from $0.2, 1.2, 2.4$ mm^{-1}. The anisotropy factor in Henyey-Greenstein scattering function is $g = 0.5$. For all performed calculations, it was assumed that the refractive index of tissues is 1.4 and the modulation frequency is $f = 100$ MHz.

The amplitude and the phase shift of the simulated data are plotted against the source-detector distance in Fig.4. The results of Hybrid Monte Carlo method are compared with the coupled RTE–DA model and Monte Carlo simulation. The black dotted curve shows results for a z_c set to $\frac{0.8}{\mu_a+\mu'_s}$, whereas the white dotted curve is for $z_c = \frac{0.5}{\mu_a+\mu'_s}$. Two values of critical depth are tested only when the scattering coefficient is the lowest. In this case (Fig.4(a)), we see that the hybrid Monte Carlo – diffusion model agrees better with the pure Monte Carlo method when the critical depth is set to a higher value. Thus it forces the Monte Carlo step of hybrid method to be longer and much avoid the failure of the diffusion approximation. For the other cases (b) and (c), the optimized critical depth is $z_c = \frac{0.5}{\mu_a+\mu'_s}$. We note that the error in both hybrid models decreases with the increasing scattering coefficient of the turbid slab. The amplitude and phase calculated with the hybrid MC method are close to those obtained with the MC method results as well as the coupled RTE–DA method in the case in which the scattering coefficient of the turbid media is 1.2 or 2.4 mm^{-1} (Fig. 4(b) and (c)).

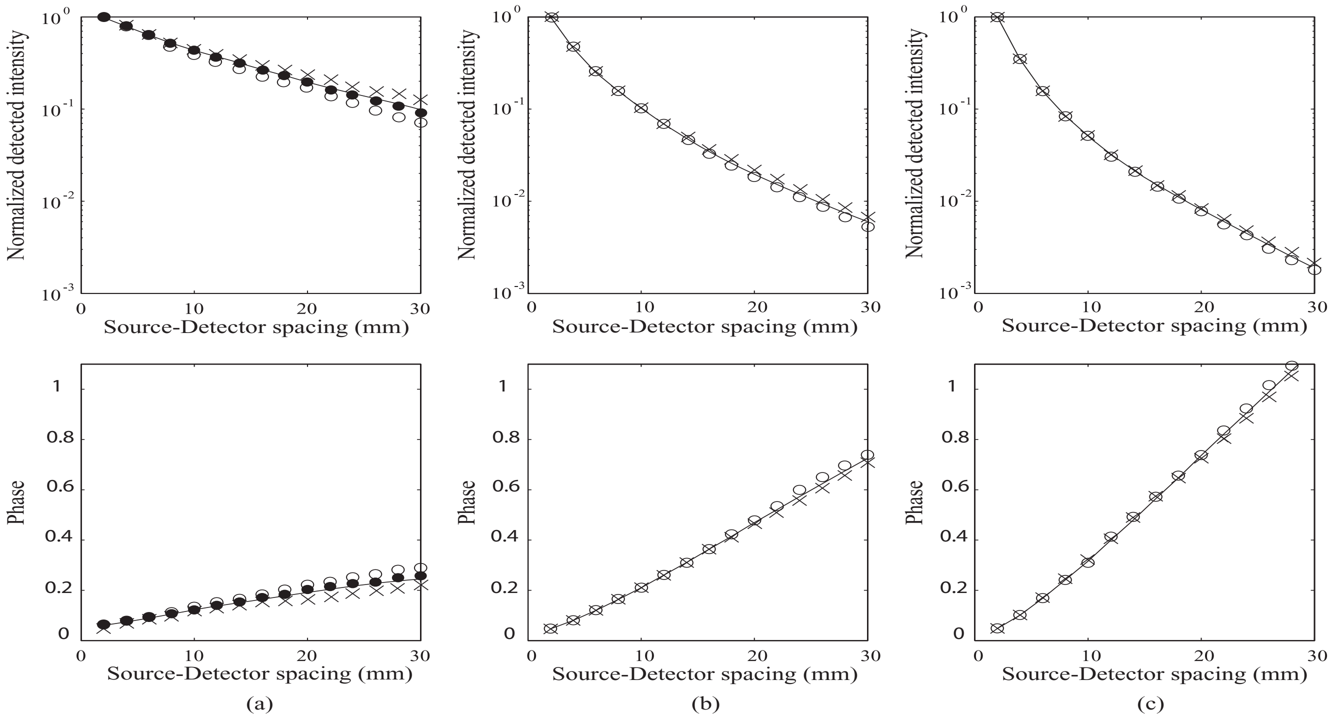

Figure 4: Comparisons between the pure MC (solid curve), the hybrid MC (dotted curves; see text) and the coupled RTE–DA (crossed curve) models. The scattering coefficient of the turbid slab was varied from (a) 0.2, (b) 1.2, (c) 2.4 mm^{-1}, while the other properties were held constant.

Table 2: Optical coefficients for the two-layered geometry, $d_1 = 10$ mm and $d_2 = 70$ mm.

	μ_a (mm^{-1})	μ'_s (mm^{-1})
Layer 1	0.017	1.75
Layer 2, 1	0.0015	0.1
Layer 2, 2	0.0015	0.6
Layer 2, 3	0.0015	1.2

In almost all applications, models have assumed homogeneous tissues. Unfortunately, this assumption is often not valid. Instead, many tissue parts have a layered structure: skin and subcutaneous fat or muscle, layers of the head above the brain. Therefore, as a second geometry, we investigated a two-layered turbid medium in order to test our hybrid models on more realistic media. In all of the simulations cases, the thickness of the first layer is 10 mm and the second one is 70 mm (Fig.3 and Tab.2). The frequency-domain reflectance amplitude and phase are computed using μ_{a1} = 0.017 mm^{-1}, μ_{s1} = 3.5 mm^{-1}, μ_{a2} = 0.0015 mm^{-1} and μ_{s2} = 0.2, 1.2, 2.4 mm^{-1}. All other properties are held constant from the previous example. The results are reported in Fig.5. To avoid grid size effects, the overall computed results reported have been performed using a bounded domain of size 80 mm x 60 mm. The characteristics of hybrid MC method are unchanged except the critical depth which is set to $(d_1 + \frac{\alpha}{\mu_{a2}+\mu'_{s2}})$ where d_1 is the thickness of the top layer and $\alpha = 0.5$ or 0.8. With this second geometry, we note the same conclusions. The amplitudes and phase shifts computed with the two hybrid models agree well with the MC method results and the quality of the hybrid simulations increase with the scattering coefficient from left to right in Fig.5. We can also note that hybrid models give good results in the vicinity of the source whereas this point is the drawback of the conventional DA. The accuracy of both hybrid models differs for the lowest-scattering media. Indeed, we can act on the critical depth to improve the hybrid Monte Carlo – diffusion model. The deeper the z_c, the better the precision but the longer the simulation time. Although the accuracy of both hybrid models is close to the MC validation

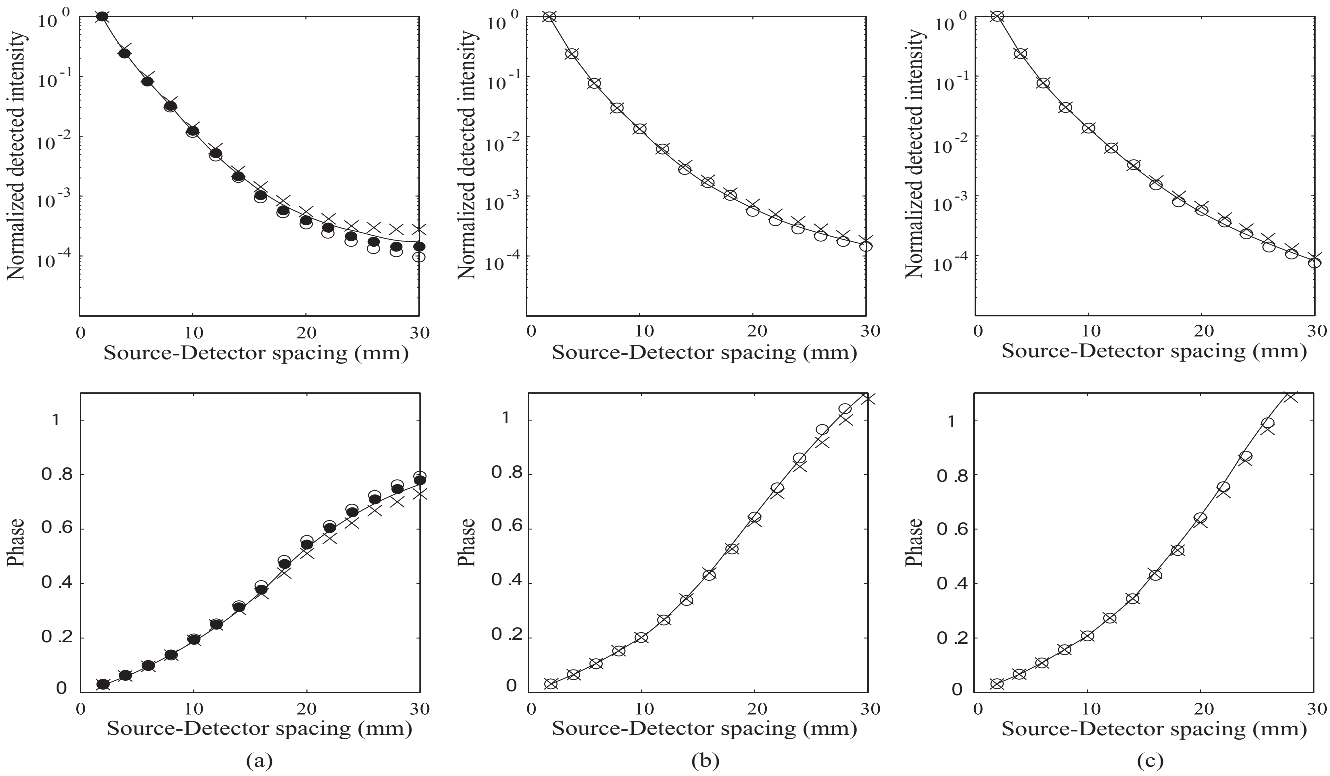

Figure 5: Amplitude and phase of detected light simulated by the pure MC (solid curve), the hybrid MC (dotted curves) and the coupled RTE–DA (crossed curve) models. The scattering coefficient of the bottom layer was varied from (a) 0.2, (b) 1.2, (c) 2.4 mm^{-1}.

method in the majority of the cases, we can discuss the computation time of each simulation. The number of photon packets that were traced in the simulation was one million for both the pure and the hybrid Monte Carlo models. This parameter influences the simulation user time. However, the computation time of the hybrid MC–DA model and of the coupled RTE–DA model are insensitive to the optical properties. In contrast, the pure Monte Carlo is very dependent on the optical coefficients values. Therefore, the simulation is computationally very expensive when the absorption coefficient is much lower than the scattering parameter because photons must travel a longer path before being totally absorbed. The average computation time for all pure MC simulations is about one hour whereas it takes a few seconds for performing hybrid models. The computation time is about from 50 s to 60 s for the coupled RTE–DA simulations whatever the geometry case, whereas the MC–DA model is performed in about 30 s for the smallest value of z_c and 120 s for the deeper one. Although the MC–DA model is optimized in C language, the coupled RTE–DA Matlab codes are not optimal, since the method is still under development, and programming the coupled model codes in C would speed them up.

4 Conclusion

In this paper, we compared different numerical approaches to solve the forward problem in biomedical optics. The light propagation was first modeled with an hybrid Monte Carlo method. The latter combines the accuracy of the statistical Monte Carlo simulations near the source and the speed of the diffusion theory distant from the laser impulsion. Then, the method was compared with the finite element solution of the coupled RTE–DA model and with pure Monte Carlo simulation. The results show that the MC–DA method is promising to rapidly investigate the distribution resulting from photon transport in multi-layered systems. Moreover, we proved that the accuracy of this model in low-scattering medium can be improved by acting on the z_c parameter even though it is a diffusion based method. Indeed, the results show that the increased critical depth causes a reduced contribution to the diffuse reflectance at the diffusion step of the MC–DA model and makes the MC step dominant that causes a better accuracy but a higher computation time. The big challenge is to find a compromise between an acceptable computational time and a good precision of results.

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