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Source of error in calculation of optical diffuse reflectance from turbid media using diffusion theory

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Abstract

Diffusion theory and similarity relations were used to calculate the optical diffuse reflectance of an infinitely narrow laser beam incident upon a semi-infinite turbid medium. The results were analyzed by comparison with the accurate results from Monte Carlo simulations. Because a large number of photon packets were traced, the variance of the results from Monte Carlo simulations was small enough to reveal the detailed defects of the diffusion theory and the similarity relations, which are broadly used in photomedicine. We demonstrated that both diffusion theory and similarity relations provide very accurate results when the photon sources are isotropic and buried more deeply than one transport mean free path in turbid media. We found that the key factor affecting the accuracy of the diffusion theory application was the conversion from the infinitely narrow laser beam to an isotropic point source in turbid media. © 2000 Elsevier Science Ireland Ltd. All rights reserved.

Keywords: Turbid media; Diffuse reflectance; Monte Carlo; Diffusion theory; Similarity relations

1. Introduction

In the field of laser-tissue interaction, there is a growing demand for accurate and fast models to theoretically predict the light distribution in turbid media with given optical properties, and to inversely deduce the optical properties from measurable quantities [1,2]. Most biological tissues, except the ocular tissues, are turbid media. One of the measurable quantities is the diffuse reflectance as a function of the distance between the observation point and the incident point of a laser beam. The diffuse reflectance is defined in this paper as the photon probability of re-emission from inside a semi-infinite turbid medium per unit surface area no matter whether the photon source is in or outside of the turbid medium. Measurements of the diffuse reflectance can be used to determine the optical properties of tissue non-invasively [3–10]. Modeling the diffuse reflectance of a turbid medium with given optical properties is a forward problem. Solving for the optical properties from the diffuse reflectance is an inverse problem. Solving the inverse problem requires solving the forward problem repetitively until the inverse problem has converged. Therefore, an efficient

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and accurate forward model is desirable to relate the diffuse reflectance to the optical properties of a turbid medium.

Monte Carlo technique [11–14] offers a flexible and accurate approach toward photon transport in turbid media. It can deal with complex geometry in a straightforward manner and can score multiple physical quantities simultaneously. The accuracy of Monte Carlo simulations has been tested with experimental results [15]. In this paper, Monte Carlo simulation results are used as the standards to check the accuracy of other theories. However, Monte Carlo simulations usually require tracing a large number of photons to get an acceptable variance due to its statistical nature. Therefore, Monte Carlo simulations are computationally expensive, especially when the absorption coefficient is much less than the scattering coefficient of the media, in which photons may propagate over a long distance before being absorbed.

Although diffusion theory [5] offers a fast approach to approximate certain physical quantities of light transport in turbid media, it is not valid near the photon source or boundary where the photon intensity is strongly anisotropic, which violates the assumption of diffusion theory. In therapeutic applications of lasers in medicine, the photon fluence near the source is the site of most intense laser-tissue interaction. This region is where diffusion theory is most inaccurate. In diagnostic and dosimetric measurements, such as the diffuse reflectance $R(r)$ as a function of the source-detector distance r, the reflectance near the source is the strongest, and therefore, can be more easily and accurately measured experimentally. Again, this region is where diffusion theory is most inaccurate.

The problem to be solved is to compute the diffuse reflectance of an infinitely narrow photon beam normally incident upon a semi-infinite homogeneous turbid medium with given optical properties. Although no photon beam is infinitely narrow, the beam may be considered infinitely narrow when its size is much less than the mean free scattering path length of the turbid medium. The diffuse reflectance of an infinitely narrow beam can be convolved to compute the response of a finite-size photon beam when the symmetry allows [12,16]. Although a real biological tissue is never infinitely wide, it can be so treated on the condition that it is much larger than the spatial extent of the photon distribution.

We will analyze the diffusion theory and the associated similarity relations [17] step by step and locate the key factor that affects the accuracy of diffusion theory. This analysis has proven to provide guidance for new-theory developments.

2. Methods

The optical properties of a turbid medium can be described using four parameters: relative refractive index n_{rel}, absorption coefficient μ_a, scattering coefficient μ_s, and anisotropy factor g. The refractive index n_{rel} is the ratio between the refractive index of the turbid medium and that of the ambient medium. The absorption coefficient μ_a is defined as the probability of photon absorption per unit infinitesimal path length. The scattering coefficient μ_s is defined as the probability of photon scattering per unit infinitesimal path length. The anisotropy factor g is the average cosine of the deflection angle from a single scattering event. The anisotropic scattering of biological tissues is usually represented [18] by a Henyey–Greenstein scattering function [19]. We will use the following optical parameters as an example: $\mu_a = 0.1$ cm^{-1}, $\mu_s = 100$ cm^{-1}, $g = 0.9$, which are typical for tissues in the visible and infrared wavelength region [20]. Only matched boundary condition ($n_{rel} = 1$) is considered in the paper.

A cylindrical coordinate system was set up for this problem [Fig. 1(a)]. The origin of the coordinate system was the point of photon incidence upon the surface. The $z = 0$ plane was on the surface of the medium, and the z-axis pointed downward into the medium. The radial coordinate and azimuthal angle were denoted by r and θ, respectively.

In the diffusion approximation of the transport equation, the diffuse photon intensity was assumed to be almost uniform in all directions [21]. The fluence rate distribution generated by a point source in an infinite turbid medium was easily solved analytically under the diffusion approximation and was given by:

$$\phi_1(r,\ \theta,\ z;\ r',\ \theta',\ z')=\frac{1}{4\pi D}\frac{\exp(-\mu_{\text{eff}}\rho)}{\rho} \quad (1)$$

where ρ was the distance between the observation point $(r,\ \theta,\ z)$ and the source point $(r',\ \theta',\ z')$:

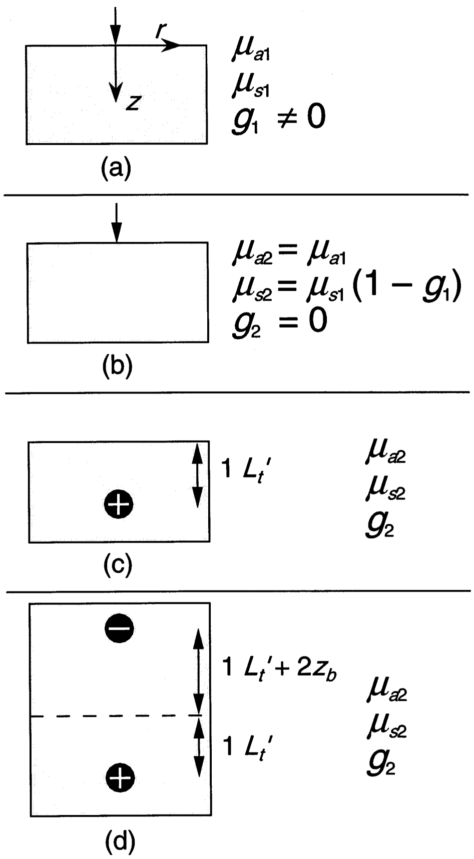

Fig. 1. Illustrations of the steps of approximation that were made to apply diffusion theory. The boxes in the figure represent turbid media. (a) An infinitely narrow photon beam incident upon the original turbid medium with the absorption coefficient μ_{a1}, scattering coefficient μ_{s1}, and non-zero anisotropy factor g_1. (b) An infinitely narrow photon beam incident upon an isotropically scattering medium with $\mu_{a2}=\mu_{a1}$, $\mu_{s2}=\mu_{s1}\ (1-g_1)$, $g_2=0$. (c) An isotropic point source $1L_t'[1\ L_t'=\mu_{s2}/(\mu_{a2}+\mu_{s2})]$ under the surface of the isotropically scattering medium. (d) An image point source was added to satisfy the boundary condition in diffusion theory. The optical parameters of the original medium in Fig. 1(a) were $\mu_{a1}=0.1\ \text{cm}^{-1}$, $\mu_{s1}=100\ \text{cm}^{-1}$, $g_1=0.9$, $n_{\text{rel}}=1$. The optical parameters of the original medium in Fig. 1(b) were $\mu_{a2}=0.1\ \text{cm}^{-1}$, $\mu_{s2}=10\ \text{cm}^{-1}$, $g_2=0$, $n_{\text{rel}}=1$.

$$\rho=\sqrt{r^2+r'^2-2rr'\cos(\theta-\theta')+(z-z')^2} \quad (2)$$

D was the diffusion constant:

$$D=\frac{1}{3[\mu_a+\mu_s(1-g)]} \quad (3)$$

and μ_{eff} was the effective attenuation coefficient:

$$\mu_{\text{eff}}=\sqrt{\mu_a/D} \quad (4)$$

The fluence rate distribution generated by a point source in a semi-infinite medium may be estimated by a linear combination of the responses for the original point source and an additional image point source, where both sources were in an infinite medium, as described by Farrell et al. [5] The added image point source was positioned to satisfy the boundary condition so that the problem for the semi-infinite medium could be converted into a problem for an infinite medium. A linear combination of Eq. (1) for the sources yielded the fluence rate of the original isotropic point source in the semi-infinite medium.

$$\begin{aligned}\phi(r,\ \theta,\ z;\ r_s,\ \theta_s,\ z_s)\\ &=\phi_1(r,\ \theta,\ z;\ r_s,\ \theta_s,\ z_s)\\ &\quad-\phi_1(r,\ \theta,\ z;\ r_s,\ \theta_s,\ -z_s-2z_b)\end{aligned} \quad (5)$$

where z_b, equal to $2D$ for a matched boundary condition, was the distance between the virtual boundary and the real boundary. The fluence rate on the virtual boundary was approximately zero.

We were interested in the diffuse reflectance from the top surface of the semi-infinite medium, which was calculated from Eq. (5) as:

$$\begin{aligned}R(r,\ 0,\ 0;\ 0,\ 0,\ z')&=D\frac{\partial\phi}{\partial z}\Big|_{z=0}\\ &=\frac{z_s(1+\mu_{\text{eff}}\rho_1)\exp(-\mu_{\text{eff}}\rho_1)}{4\pi\rho_1^3}\\ &\quad+\frac{(z+4D)(1+\mu_{\text{eff}}\rho_2)\exp(-\mu_{\text{eff}}\rho_2)}{4\pi\rho_2^3}\end{aligned} \quad (6)$$

where ρ_1 was the distance between the observation point $(r,\ 0,\ 0)$ and the source point $(0,\ 0,\ z')$ and ρ_2 was the distance between the observation point $(r,\ 0,\ 0)$ and the image source point $(0,\ 0,\ z'+4D)$.

The real problem that we wanted to solve was the diffuse reflectance of an infinitely narrow photon beam normally incident upon a semi-infinite turbid medium with anisotropic scattering. In order to use the established diffusion theory for an isotropic point source, the infinitely narrow photon beam had to be converted into an isotropic point source, or into a spatial distribution of isotropic point sources. Farrell et al. [5] converted an infinitely narrow photon beam into an isotropic point source which was 1 transport mean free path L_t' below the surface, where $L_t' = 1/[\mu_a + \mu_s(1-g)]$. The strength of the point source was the original source strength multiplied by the transport albedo a', where $a' = \mu_s(1-g)/[\mu_a + \mu_s(1-g)]$.

In this diffusion theory, there were several steps of approximation (Fig. 1). Initially, similarity relations [17] were invoked to convert the anisotropic scattering [Fig. 1(a)] of the medium into isotropic scattering [Fig. 1(b)]. Secondly, the infinitely narrow photon beam was converted into an isotropic point source at a depth of 1 L_t' below the surface [Fig. 1(c)]. Thirdly, the boundary was removed after an image source was added above the surface at the position $z = -(1L_t' + 2z_b)$. This step allowed the problem to be treated as an infinite medium with a solution that equaled the linear combination of the responses to these two sources.

The Monte Carlo technique was used to simulate the diffuse reflectance in each of the above steps [12,14]. Because the implicit photon capturing technique [22] was used during the Monte Carlo simulation, a photon packet with an initial weight of unity was launched perpendicularly to the surface along the z-axis for the problem in Fig. 1(a) and (b) and isotropically for the problem in Fig. 1(c). Then, a step size s was chosen statistically using:

$$s = \frac{-\ln(\xi)}{\mu_a + \mu_s} \tag{7}$$

where ξ was a random number equidistributed between 0 and 1 ($0 < \xi \leq 1$). The photon packet lost its weight partially at the end of each step due to absorption. The amount of weight loss was the photon weight at the beginning of the step multiplied by $(1-a)$, where a was the albedo $\mu_s/(\mu_a + \mu_s)$. The photon with the remaining weight was scattered. A new photon direction was statistically determined by the Henyey–Greenstein phase function according to the anisotropy factor g. A new step size was then generated by Eq. (7), and the process was repeated. When the photon weight was less than a preset threshold (10^{-4} in this study), Russian roulette was used to determine whether the photon should be terminated or propagated further with an increased weight. If the photon packet crossed the surface boundary into the ambient medium, the photon weight contributed to the diffuse reflectance $R(r)$. Multiple photon packets were used to obtain statistically meaningful results. In this study, one million photon packets were used in the Monte Carlo simulations.

3. Results

The diffuse reflectance $R(r)$ as a function of r, the distance between the observation point and the photon incident point, that was calculated using the diffusion theory was accurate only when the distance r was $> 1L_t'$ ($1L_t'$ was about 0.1 cm for this simulation) but inaccurate when the distance was small (Fig. 2).

Figs. 3–5 illustrate the deviations caused by each of the approximations listed above. Curves A, B, and C in the figures were the results from the Monte Carlo simulations that yielded the diffuse reflectance $R(r)$ versus the distance r. Curve D was from the diffusion theory. In Fig. 3, we compare the results obtained using anisotropic ($g = 0.9$) and isotropic ($g = 0$) scattering functions, where the reduced scattering coefficient $\mu_s(1-g)$ was conserved [Fig. 1(a) vs. (b)]. The relative error was $> 100\%$ around $r = 0$, was $\sim$ 20% near $r = 2L_t' = 0.2$ cm, and decreased with an increased distance.

In Fig. 4 we compare the results obtained for an infinitely narrow photon beam at the surface and an isotropic point source at a depth of $1L_t'$ for the medium of isotropic scattering [Fig. 1(b) vs. (c)]. This transformation approximated the penetration of the infinitely narrow photon beam

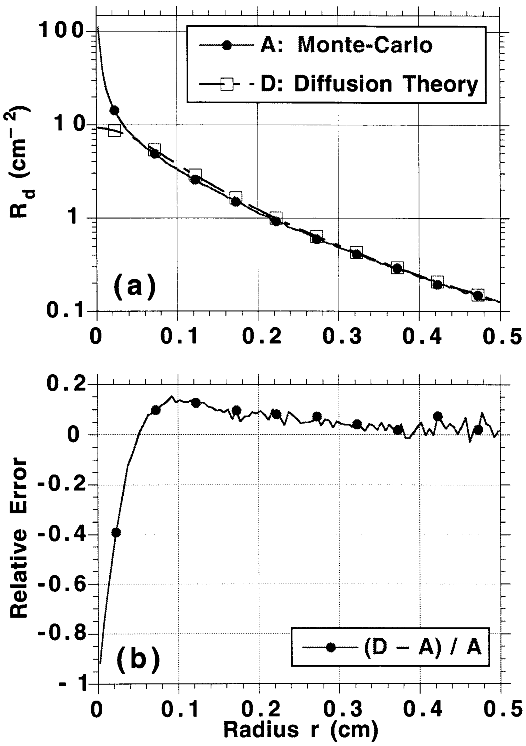

Fig. 2. (a) The diffuse reflectance of an infinitely narrow photon beam incident upon a semi-infinite turbid medium. Curve A was from the Monte Carlo simulation for the problem in Fig. 1(a). Curve D was from the diffusion theory for the problem in Fig. 1(d) after the three steps of approximation. (b) The relative error between the two curves in (a), which was the difference between curves D and A divided by curve A. The optical properties were given in the caption of Fig. 1.

by a single isotropic point source at $z = 1L_t'$. Such a transformation caused a severe underestimation of $R(r)$ near $r = 0$.

In Fig. 5 we compare the results obtained for a single isotropic point source in a semi-infinite medium using the Monte Carlo simulation and the results for a pair of isotropic point sources in an infinite medium using the diffusion theory [Fig. 1(c) vs. (d)]. There was very little systematic difference between the two calculations.

Farrell et al. [5] also used an exponentially decaying line source perpendicular to the surface to convert the infinitely narrow photon beam. They reported that the result, which was a linear combination of all the point-source responses along the source line, was not satisfactory. We found that although the diffusion approximation was acceptable when the isotropic point source was far away from the medium surface as demonstrated in Fig. 5, it became unacceptable if the source approached the surface (Fig. 6). We compared the results from the Monte Carlo simulation and the diffusion theory for the problems in Fig. 1(c) and (d), respectively, except that the point source was $0.1L_t'$ or $0.01L_t'$ instead of $1L_t'$ below the surface. We found that, as expected, the diffusion theory approximation degraded when the point source was closer to the surface. This is because that the boundary condition was not well satisfied using the image source as the photon source approached the surface and the diffusion theory itself performed poorly near the point source.

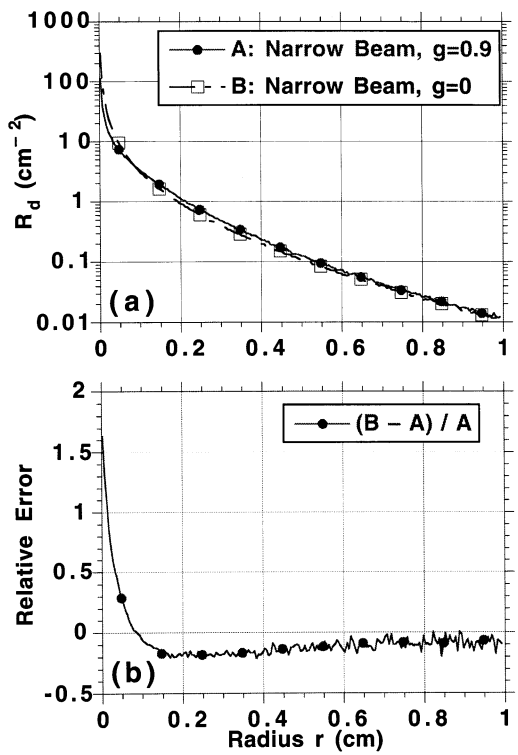

Fig. 3. (a) Comparison between the anisotropically [Fig. 1(a)] and isotropically [Fig. 1(b)] scattering media calculated using the Monte Carlo technique in terms of the diffuse reflectance and (b) the relative error as a function of the radius r. The optical properties were given in the caption of Fig. 1.

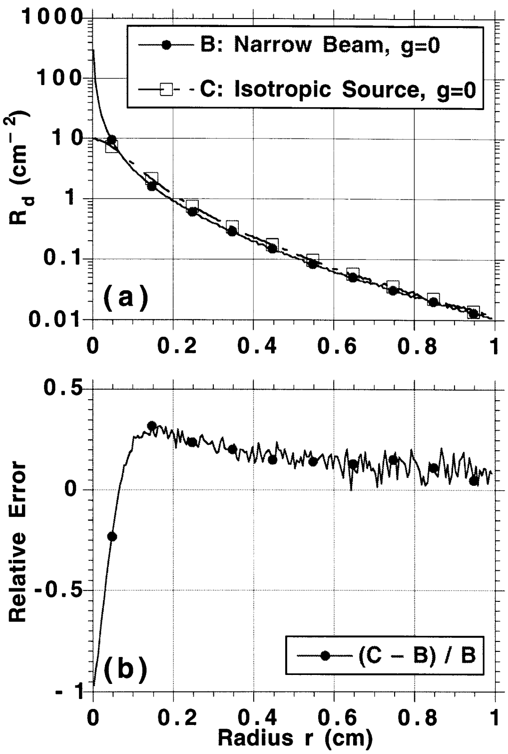

Fig. 4. (a) Comparison between an infinitely narrow laser beam [Fig. 1(b)] and an isotropic point source [Fig. 1(c)] calculated using the Monte Carlo technique in terms of the diffuse reflectance from an isotropically scattering medium and (b) the relative error as a function of the radius r. The optical properties were given in the caption of Fig. 1.

Regarding the similarity relations, although they yielded considerable error in $R(r)$ when applied for photons originating near the surface as demonstrated in Fig. 3, they were acceptable when the photons originate deep inside the medium [17]. To demonstrate this point, we computed the diffuse reflectance from an isotropic point source $1L_t'$ below the surface with isotropic scatterings [as in Fig. 1(c)] and anisotropic scatterings using the Monte Carlo simulation, where the optical parameters of the two cases were governed by similarity relations. The results from the two calculations were close to each other (Fig. 7).

4. Conclusions and discussion

In the diffusion theory, most of the error was caused by converting the infinitely narrow photon beam incident upon the anisotropically scattering medium to an isotropic point source at a depth of $1L_t'$ inside an isotropically scattering medium. Little error was caused by converting the single source in a semi-infinite medium to double sources in an infinite medium.

In order to use diffusion theory accurately, we must accurately convert the infinitely narrow photon beam into isotropic photon sources that must be sufficiently deep in the medium, e.g. $1L_t'$ deep. Furthermore, the absorption coefficient μ_a should be much less than the reduced scattering coeffi-

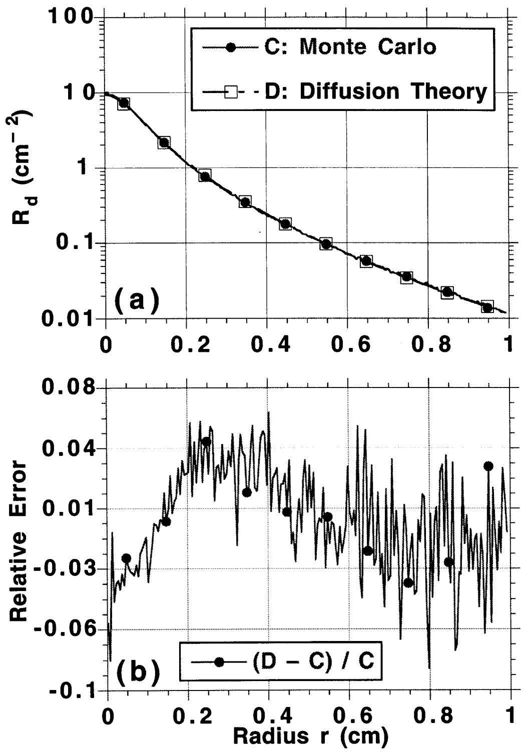

Fig. 5. (a) Comparison between an isotropic point source in a semi-infinite turbid medium [Fig. 1(c)] and a pair of isotropic point sources in an infinite turbid medium [Fig. 1(d)] in terms of the diffuse reflectance and (b) the relative error as a function of the radius r. Curves C and D were based on the Monte Carlo technique and the diffusion theory, respectively. The optical properties were given in the caption of Fig. 1.

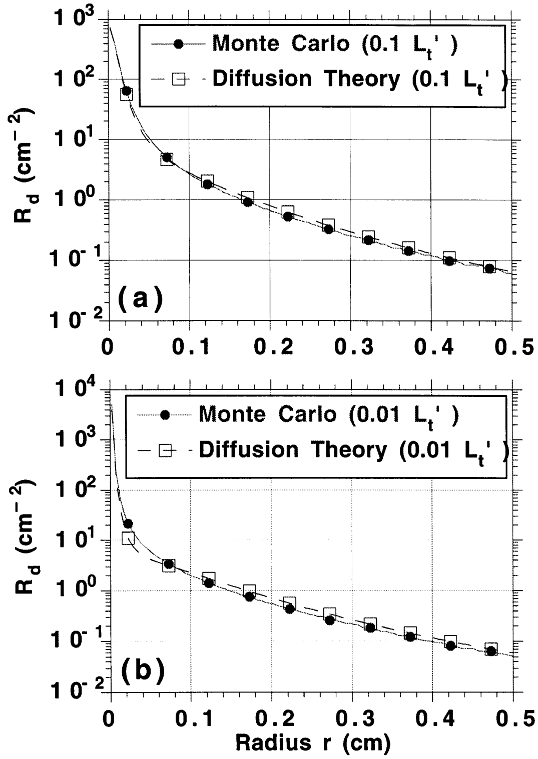

Fig. 6. Comparison between the Monte Carlo technique and the diffusion theory in terms of the diffuse reflectance as a function of the radius r. An isotropic photon source was buried (a) $0.1L_t'$ or (b) $0.01L_t'$ below the isotropically scattering semi-infinite turbid medium. The optical properties of the semi-infinite medium were given in the caption of Fig. 1.

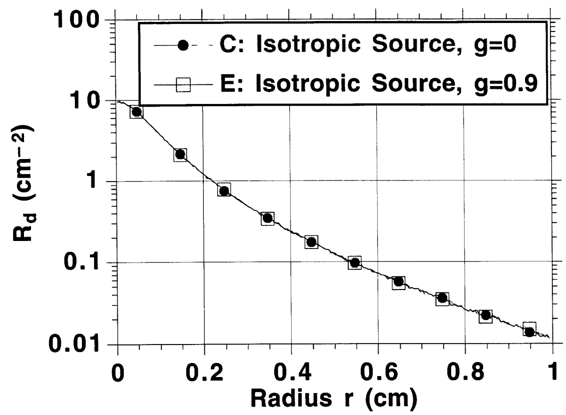

Fig. 7. Comparison between two turbid media whose optical properties were related by similarity relations in terms of the diffuse reflectance computed with the Monte Carlo technique due to an isotropic point source $1L_t'$ deep as a function of the radius r. The optical properties were: $\mu_a = 0.1$ cm^{-1}; $\mu_s = 10$ cm^{-1}; $g = 0$, $n_{rel} = 1$ for curve C and $\mu_a = 0.1$ cm^{-1}; $\mu_s = 100$ cm^{-1}; $g = 0.9$, $n_{rel} = 1$ for curve E.

cient $\mu_s(1-g)$ as required by the diffusion approximation.

It was demonstrated that the similarity relations can be used with a good accuracy in the calculation of diffuse reflectance when they are applied for photon sources deep inside the turbid media, e.g. $1L_t'$ deep.

These conclusions have sparked the development of a new theory called the hybrid model combining the Monte Carlo simulations and the diffusion theory [23]. The Monte Carlo simulation, while collecting some diffuse reflectance due to the near-surface scattering, was used initially to propagate photons to sufficient depths into the turbid media so that diffusion theory could be applied with a good accuracy. Deep photons were then converted into isotropic photon sources by means of similarity relations. Diffusion theory was then used to compute the diffuse reflectance, due to the distributed isotropic photon sources. The final diffuse reflectance was the sum of the two parts. The hybrid model combined the accuracy advantage of the Monte Carlo simulations and the speed advantage of the diffusion theory.

In this research, only matched boundaries between the ambient and the turbid media were considered. In the future studies, mismatched boundaries will be investigated. But the main conclusions from this research are expected to hold.

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