Energy Conversion and Management xxx (2008) xxx–xxx

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

A frequency-based numerical approach for unsteady radiative transfer in participating media

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ARTICLE INFO

Article history:
Received 11 July 2007
Accepted 17 December 2007
Available online xxxx

Keywords:
Radiative transfer
Biomedical imaging
Tomography
Pulsed laser
Frequency-based numerical method

ABSTRACT

The one-dimensional transient radiative transfer problem in the Cartesian coordinate system – an absorbing and scattering medium illuminated by a short laser pulse – is solved by the use of a discrete ordinates–finite volume method. Previous works have shown that the original numerical approach, based in the space–time domain, induces transmitted flux emerging earlier than the minimal time required by the radiation to leave the medium. Therefore, a frequency-based numerical method is formulated, implemented, and validated in this paper. Results for transmittances are accurate, without physically unrealistic behaviors at early time periods. However, the frequency-dependent approach is computationally expensive; it requires approximately five times more computational time than its temporal counterpart. Ongoing research is devoted to the optimization of these CPU requirements.

1. Introduction

The interest for transient radiative transfer has recently increased, mainly because of numerous possible uses of short pulse lasers in a wide variety of engineering applications but especially in biomedical imaging where non-intrusive tools are needed at low costs and without side effects [1–9]. Optical diagnosis of absorbing and scattering media using temporal distributions of transmittance and/or reflectance remains a promising application of transient radiative transfer [1–10].

Transient effects associated with radiation heat transfer can be neglected when the time needed by the photons to leave a medium is shorter than the period of variation of the radiative source, which is the case in most engineering applications. However, a radiative flux emitted in a short time scale (from picosecond to femtosecond), such as a pulsed laser, involves non-negligible unsteady effects. Therefore, a typical transient radiative transfer problem arises when an absorbing and scattering medium is illuminated by a short laser pulse, for which the duration is of the same order of magnitude, or less, than the time needed by the radiation to leave the medium [1].

A wide variety of methods have been developed in order to solve the time-dependent radiative transfer equation. Among these methods: the Monte Carlo (MC) formulations [12–15], the classical spherical harmonics [1], and the modified $MP_{1/3}A$ [16], the two-flux approaches [1], the radiation element method [17], the discrete ordinates approaches [18–24], the integral formulation [25] and, more recently, a backward method of characteristics [26].

In this paper, a discrete ordinates–finite volume (DO–FV) approach is retained, where DO and FV refer to the directional and spatial discretizations, respectively. The main drawback of a DO–FV approach, based in the time domain, is that radiative fluxes are transmitted earlier than the minimal time required by the radiation to leave the medium. This has been widely reported in the literature [16,19,22–24] and it is caused mainly by the interdependence between the spatial and temporal discretizations, and also by the numerical approximations embedded within the application of an interpolation scheme.

In order to avoid early transmitted radiation, some researchers [16,19,27] have proposed using high order spatial interpolation schemes; this has been tested by the authors in their last contribution to the ICTEA [22]. Despite the implementation of a second-order Lax–Wendroff scheme, coupled with a Van Leer or a Superbee flux limiter, the physically unrealistic behavior were still present. It has been concluded that the non-physical transmitted fluxes cannot be totally avoided with an approach based in the space–time domain, but only minimized with the use of high-order schemes.

On the other hand, in order to assess the use of the diffusion approximation for the solution of transient radiation transport problems, Elaloufi et al. [28] solved the time-dependent radiative transfer equation in the space–frequency domain with a DO method. This provided the incentive for the present research work that pertains to the solution of the [illegible]ative transfer equation (RTE) in the space–frequency domain.

The problem under consideration and the associated assumptions are succinctly described in the second section. The third part

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0196-8904/$ - see front matter © 2008 Published by Elsevier Ltd.
doi:10.1016/j.enconman.2007.12.034

Nomenclature

a	anisotropy factor (–)
c	speed of electromagnetic waves in the medium (ms^{-1})
H	Heaviside function (–)
i	complex constant (–1)$^{1/2}$
I	intensity (Wm^{-2} sr^{-1} μm^{-1})
j	spatial node (–)
k	frequency step (–)
m	discrete direction (–)
n	temporal step (–)
Re	real part of a complex number (–)
S_c	source term (Wm^{-2} μm^{-1})
t	time (t)
t^*	dimensionless time (–)
T	hemispherical transmittance (–)
w_m	discrete solid angle, weight of a numerical quadrature (–)
z	spatial coordinate (m)

Greek symbols

β	extinction coefficient (m^{-1})
θ	polar angle (rad)
μ	direction cosine
τ	optical depth
σ	scattering phase function
ω	albedo for single scattering
$\hat{\omega}$	time-dimensionless angular frequency (pulsation)

Subscripts

0	incident collimated beam
c	collimated component
d	diffuse component
j	spatial node
$j \pm 1/2$	the boundary of a control volume
L	medium thickness
p	pulse

Exponents

′	other directions
ˆ	frequency-dependent quantity
k	discrete frequency step
m	discrete direction
n	temporal step

of the paper is devoted to the theoretical and numerical formulation of the frequency-dependent method. This approach is then applied to solve two one-dimensional transient radiative transfer problems, and results are compared with those obtained previously by the authors from time-based techniques [22,23,29] and with those available in the literature.

2. Problem description and assumptions

Throughout this paper, the following assumptions apply: (1) the medium is a plane–parallel semi-infinite layer of thickness z_L; (2) the layer is composed of an non-emitting, absorbing and scattering homogeneous medium, with a relative unit refractive index; (3) radiative properties are calculated at the central wavelength of the pulse's spectral bandwidth and, consequently, reference to wavelength is omitted in the notations; (4) scattering is assumed to be independent (valid although the medium is a semitransparent solid); (5) boundaries are transparent; (6) the layer is subject to a collimated short square pulse of radiation at normal incidence (the problem is azimuthally symmetric); (7) a pure transient radiative transfer regime is considered, that is, the pulse width is less than characteristic time for the establishment of any other phenomenon [1]; and (8) local thermodynamic equilibrium does not break down although the transients are fast due to the brief period of emission of the pulse, particles are assumed to adjust to new conditions during the transient.

This typical one-dimensional transient radiative transfer problem is schematically depicted in Fig. 1.

The fraction of the incident collimated radiation beam which is not scattered crosses the medium in a straight line. Therefore, for this fraction of the beam, the time required to leave the medium is the shortest that is $t_L = z_L/c$. For an optically thick and highly scattering medium, an important part of the photons are scattered in all directions (travel paths L_1 and L_2). Therefore, the time required by these photons to leave the medium at the boundary $z = z_L$ is necessarily greater than t_L, since the traveling distances are longer. This means that the total duration of the transmitted radiative flux at the boundary $z = z_L$ (called the transmittance) is longer than the duration of the pulse. This transmitted signal is dependent on the radiative properties of the medium, since its duration and shape are dependent on the traveling paths of the photons inside the medium. In turn, the traveling paths are directly related to the absorption and scattering coefficients. Therefore, the analysis of temporal distributions of transmittance could be used for some meteorological applications [1,20,29]. A similar conclusion holds with respect to temporal distributions of the reflectance.

3. Solution in the space–frequency domain

3.1. Mathematical models

Since the problem deals with collimated irradiation, the most convenient approach to fulfill this need for a mathematical solution is to consider a separate treatment of the diffuse-scattered component (I_d) of the radiative intensity. Variations of the collimated intensity (I_c) are simply described by a spatial exponential decay and a temporal term originating from the propagation of the pulse [19,26].

The transient radiative transfer equation (TRTE) describes spatial and temporal variations of the diffuse component of the intensity along the direction μ in a participating medium [9,13,14]. Using dimensionless time ($t^* = \beta ct$) and optical depth ($\tau = \beta z$) as variables, the one-dimensional TRTE is written as follows [30]:

$$\frac{\partial I_d(\tau,\mu,t^*)}{\partial t^*} + \mu\frac{\partial I_d(\tau,\mu,t^*)}{\partial \tau} = -I_d(\tau,\mu,t^*) + \frac{\omega}{2}\int_{-1}^{1} I_d(\tau,\mu',t^*)\Phi(\mu',\mu)\mathrm{d}\mu' + S_c(\tau,\mu,t^*) \quad (1)$$

The first and second terms on the right-hand side of Eq. (1) represent, respectively, the attenuation by absorption and scattering, and the reinforcement due to the scattering of the diffuse part of intensity. In the particular case of a square pulse of dimensionless duration t_p^*, the radiation source term S_c, due to the scattering of the collimated intensity, is given by [31,32]

$$S_c(\tau,\mu,t^*) = \frac{\omega}{4\pi} I_0 \exp(-\tau)[H(t^* - \tau) - H(t^* - t_p^* - \tau)]\Phi(1,\mu) \quad (2)$$

In post-treatment, the hemispherical transmittance is calculated and can be written as

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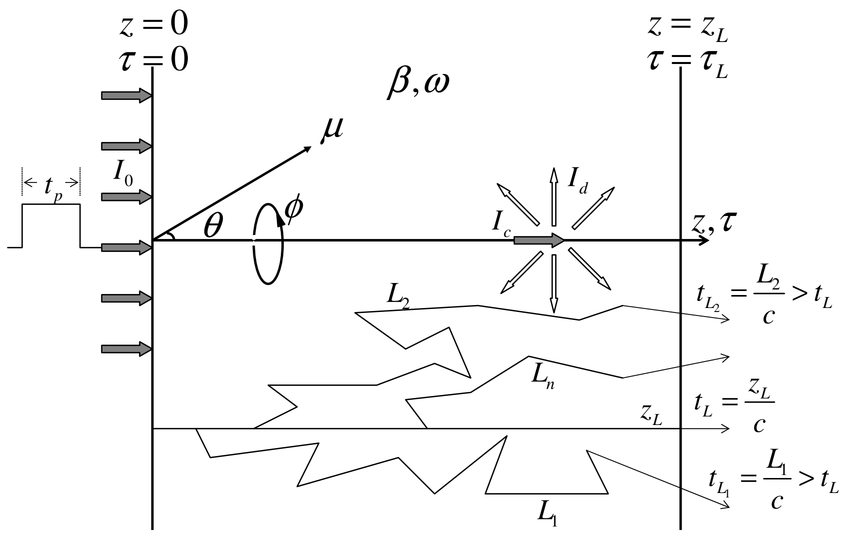

Fig. 1. Schematic of the unsteady problem.

$$T(t^*)=\frac{2\pi\int_0^1 I_d(\tau_L,\mu,t^*)\mu\,d\mu+I_c(\tau_L,t^*)}{I_0} \tag{3}$$

Since the objective is to solve the transient radiative transfer problem in the space–frequency domain, all temporal variables have to be transformed into frequency-dependent variables applying a temporal Fourier transform (FT) of the intensity [30]

$$I(\tau,\mu,t^*)=\int_{-\infty}^{\infty}\widehat{I}(\tau,\mu,\hat{\omega})\exp(i\hat{\omega}t^*)\,d\hat{\omega} \tag{4}$$

where $\hat{\omega}$ is the angular frequency deriving from the dimensionless time variable $t^*=\beta ct$, and τ is the optical depth ($\tau=\beta z$). Inversely the frequency-dependent intensity can be written as the FT of the time-dependent intensity. The time-dependent Fourier analysis applied to the TRTE leads to

$$\mu\frac{d\widehat{I}_d(\tau,\mu,\hat{\omega})}{d\tau}=-(1+i\hat{\omega})\widehat{I}_d(\tau,\mu,\hat{\omega})+\frac{\omega}{2}\int_{-1}^{1}\widehat{I}_d(\tau,\mu',\hat{\omega})\Phi(\mu',\mu)\,d\mu'+\widehat{S}_c(\tau,\mu,\hat{\omega}) \tag{5}$$

where the frequency-dependent intensity $\widehat{I}_d(\tau,\mu,\hat{\omega})$ and $(1+i\hat{\omega})$ are complex numbers. The first and second terms of the right-hand side of Eq. (5) represent, respectively, the attenuation by absorption and scattering and the reinforcement due to the scattering of the diffuse part of intensity. This equation has the form of a steady-state radiative transfer equation and is called the complex radiative transfer equation (CRTE). The source term $\widehat{S}_c$ originating from the scattering of the collimated intensity is determined from a particular solution of Eq. (5) without scattering sources [30]

$$\widehat{S}_c(\tau,\mu,\hat{\omega})=\frac{\omega}{4\pi}\widehat{I}_0(\hat{\omega})\exp[-\tau(1+i\hat{\omega})]\Phi(1,\mu) \tag{6}$$

where $\widehat{I}_0(\hat{\omega})$ is obtained from the temporal Fourier analysis of the incident pulse; this is schematically depicted in Fig. 2.

From the above statement, it is concluded that the solution of a transient radiative transfer problem can be obtained by solving the CRTE for each angular frequency contained in the temporal Fourier decomposition of the pulse.

3.2. Numerical formulation

A DO–FV approach is used in order to solve the transient radiative transfer problem in the space–frequency domain. For a given

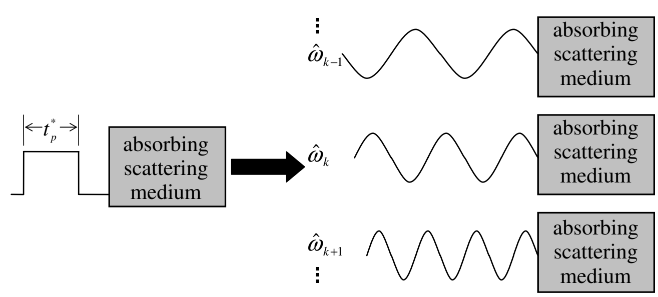

Fig. 2. Shift from the space–time to the space–frequency domain.

angular frequency $\hat{\omega}$, a steady-state radiation transport problem is solved by calculating the frequency-dependent intensities on the J nodes and M directions of the spatial and directional discretizations, respectively. Then, integrating the CRTE over a control space $\Delta\tau_j w_m$ yields

$$\widehat{I}_j^{m,k}=\frac{(-\mu_m/\Delta\tau_j)\left(\widehat{I}_{j+1/2}^{m,k}-\widehat{I}_{j-1/2}^{m,k}\right)+(\omega_j/2)\sum_{m'=1}^{M}w_{m'}\widehat{I}_j^{m',k}\Phi_j^{m'm}+\widehat{S}_{c_j}^{m,k}}{1+i\hat{\omega}_k} \tag{7}$$

where $\widehat{I}_j^{m,k}$ is the frequency-dependent intensity at node j, in direction m, and at frequency k, corresponding to the discrete pulsation $\hat{\omega}_k$ for which the CRTE is solved. The variables $I_{j\pm1/2}^{m,n}$ are the intensities at the boundaries of the control volume surrounding the node j. The subscript d, referring to the diffuse component of intensity, is omitted for more clarity.

To solve Eq. (7), one needs to relate the value of the intensity at control volume boundaries ($j\pm1/2$) – for a specific direction and frequency – to the nodal values $(\ldots,j-1,j,j+1,\ldots)$, by choosing an appropriate spatial interpolation scheme. In this work, a first-order upwind scheme is sufficient, since the CRTE is a steady-state equation.

Eq. (7) is then solved, for a specific frequency k, for each node j and in each direction m of the spatial and angular discretizations, respectively. An iterative scheme, based upon the convergence of the source term due to the scattering of the diffuse part of intensity, is used [24]. Stability and consistence of the numerical formulation were ensured.

In order to determine the frequencies for which the CRTE is solved, a temporal FT is applied on the incident square pulse

$$I_0^k = I_0\left(\frac{\sin\hat{\omega}_k t_p^*}{\hat{\omega}_k} - \mathrm{i}\frac{1-\cos\hat{\omega}_k t_p^*}{\hat{\omega}_k}\right) \tag{8}$$

The K relevant angular frequencies are selected by calculating Eq. (8) for a series of discrete pulsations $\hat{\omega}_k$. A graphical representation of the real and imaginary parts of I_0^k, as a function of $\hat{\omega}_k$, allows one to find the threshold angular frequencies, $\hat{\omega}_{-K/2}$ and $\hat{\omega}_{K/2}$, for which the CRTE has to be solved (i.e. frequencies below and above which the real and imaginary parts of I_0^k vanish). The angular frequency discretization $\Delta\hat{\omega}_k$ is determined by performing a numerical sensitivity analysis.

Finally, the time-dependent intensities have to be recovered from the frequency-dependent intensities. This is done by applying an inverse Fourier transform (IFT) on the frequency-dependent intensities

$$I_j^{m,n} = \mathrm{Re}\left\{2\sum_{k=0}^{K/2}\frac{1}{K}\exp(\mathrm{i}\hat{\omega}_k t_n^*)\widehat{I}_j^{m,k}\right\} \tag{9}$$

Eq. (9) implies that the frequency-dependent intensities can be calculated and summed only for the $K/2$ relevant angular frequencies (symmetry of the summation) in order to determine the time-dependent intensity at a given instant t_n^*. Unlike a space–time approach, the determination of the intensity at instant t_n^* does not require the knowledge of intensities at $0, t_1^*, t_2^*, \ldots, t_{n-1}^*$.

The principal steps to solve the transient radiative transfer problem in the space–frequency domain are summarized as: (1) the temporal FT of the pulse is first calculated; (2) the relevant frequencies are determined; (3) a CRTE is solved for each selected angular frequency; and (4) an IFT is applied in order to derive time-dependent intensities. It is worth noting that this formulation is an evolution of numerous previous formulations proposed in the past 15 years in the context of steady thermal radiative transfer in enclosures combined with fluid flow and convective heat transfer.

4. Results and discussions

Before any results were proposed for publication using the implemented formulation, tests were carried-out to ensure grid independent, stable converged solutions.

Two typical transient radiative transfer problems are solved in this section; in both cases, the absorbing and scattering medium is illuminated by a square pulsed collimated radiation beam of unit intensity ($I_0 = 1$) and unit dimensionless duration ($t_p^* = 1$) on its boundary $\tau = 0$ [14]. When the medium is anisotropically scattering, the linear anisotropic phase function is considered ($\Phi(\mu', \mu) = 1 + a\mu\mu'$). In post-treatment, the temporal hemispherical transmittance is calculated from the time-dependent intensities [14].

The numerical codes are written in *FORTRAN* and have originally been compiled with the software Microsoft Developer Studio – Fortran PowerStation 4 on a PC Pentium III of 600 MHz.

4.1. Optically thick and highly scattering media

In this first problem, the optical thickness of the medium is $\tau_L = 10$ while the scattering albedo is $\omega = 0.998$. The transmittance is calculated for three types of scattering media: isotropic ($a = 0$), highly forward scattering ($a = 0.9$), and highly backward scattering ($a = -0.9$). For this problem, 100 spatial nodes and 10 directions (equal weights polar quadrature) are sufficient to discretize the spatial and directional domains; no significant improvement of the results has been observed beyond these thresholds.

Also, the temporal FT of the square pulse allows the determination of pulsations for which the CRTE has to be solved (from -16π to 16π, except $\hat{\omega}_k = 0$). A preliminary parametric analysis permitted the identification of an optimal angular frequency discretization ($\Delta\hat{\omega}_k = 3\times10^{-4}\pi$).

Transmittances obtained by solving the CRTE with a DO–FV method are reported in Fig. 3. It is important to note that since the optical thickness (τ_L) of the slab is 10, the minimal dimensionless time required by the radiation to leave the medium (t_L^*) is also 10.

The sharp diminution of transmittance at $t^* = 11$, followed by an increase, is due to the fact that the collimated component of intensity has left the medium (square pulse of dimensionless duration $t_p^* = 1$). A highly forward scattering medium ($a = 0.9$) leads to a higher maximum of transmittance, since this phase function tends to throw the scattered photons at the boundary $\tau = \tau_L$. On the other hand, a highly backward scattering phase function ($a = -0.9$) produces longer travel paths of the scattered photons, leading to a weaker maximum of transmittance. For a longer period of time, the transmittance is higher for the backward scattering phase function (from $t^* \approx 85$) due to a more important photons retention. Therefore, the transmittance vanishes more quickly when $a = 0.9$.

Fig. 3 clearly indicates that for a large time scale (from 0 to 100), results from the frequency-dependent method are in good agreement with those obtained from a MC formulation, even at early time periods (i.e. near t_L^*).

In order to analyze more precisely the relative accuracy of the frequency domain approach, the transmittances obtained from this method are compared at early time periods with those obtained with a first order exponential scheme [22], the Van Leer flux limiter [23], and the Superbee flux limiter [23]. Only results (Fig. 4) for $a = 0.9$ are shown, since early transmitted radiation becomes more important as the medium is highly forward scattering.

Fig. 4 shows that no flux is transmitted before $t_L^* = 10$ only with the frequency-dependent method, since the problem associated with the interdependence between the spatial and temporal discretizations is avoided.

It can be concluded that, from a strict point of view of accuracy, the frequency-dependent approach is superior than solving directly the TRTE in the space–time domain, since the transmittance begins exactly at the dimensionless time $t^* = 10$. Even after this instant, the approaches give different results, and converged to the same values approximately between $t^* = 10$ and $t^* \approx 12$. However, the temporal resolution of the available MC results [15] is insufficient to conclude about this divergence.

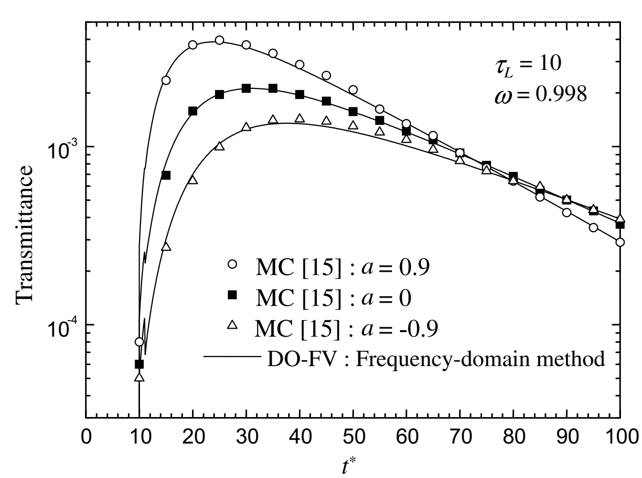

Fig. 3. Temporal distribution of hemispherical transmittance; comparison between the frequency domain approach and a MC formulation [15].

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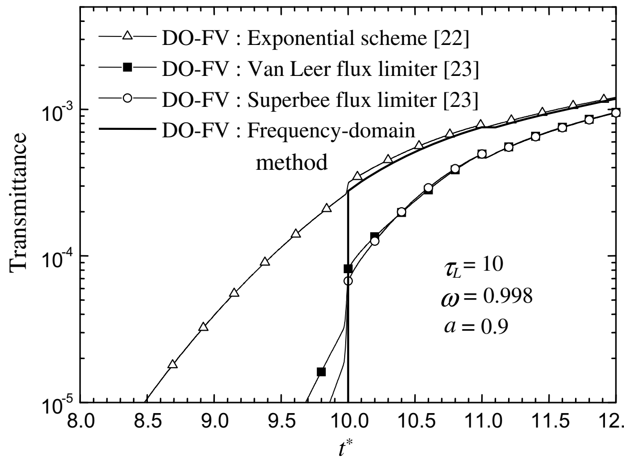

Fig. 4. Temporal distribution of hemispherical transmittance; comparison between the Van Leer flux limiter [23], the Superbee flux limiter [23], the exponential interpolation scheme [22], and the frequency domain method at early time periods.

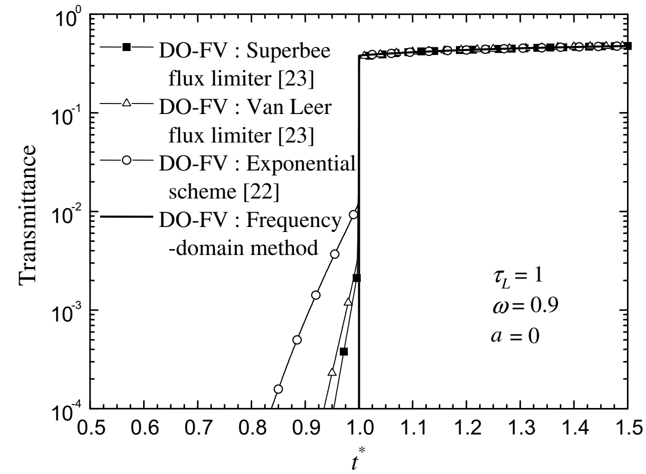

Fig. 6. Temporal distribution of hemispherical transmittance; comparison between the Van Leer flux limiter [23], the Superbee flux limiter [23], the exponential interpolation scheme [22], and the frequency domain method at early time periods.

The CPU times associated with the different methods are presented in Table 1 and have been compiled for the case of an isotropic scattering medium ($a = 0$). The frequency-dependent approach is time consuming: a large number of frequencies is required to model a square pulse, and the shift from the space–frequency to the space–time domain (IFT) constitutes a supplementary computational step, compared to the direct solution of the TRTE. For this particular problem, the frequency-dependent method requires approximately five times more CPU time than solving the problem in the space–time domain with a Superbee flux limiter [23].

Table 1
CPU times associated with different time-based approaches and the frequency-based methods for problem 1

Resolution methods	CPU time (s)	Relative CPU time (Superbee flux limiter) [–]
Time domain approach, exponential scheme	156	0.60
Time domain approach, Van Leer flux limiter	238	0.91
Time domain approach, Superbee flux limiter	262	1
Frequency domain approach	1343	5.13

4.2. Medium of unit optical thickness and variable scattering albedo

In this second problem, the optical thickness of the medium is fixed at $\tau_L = 1$ while the scattering albedo ω is variable (0.25, 0.50, 0.75 and 0.90). In all cases, the medium is isotropically scattering ($a = 0$). This second test problem has been compared [24] with a DO approach coupled with the piecewise parabolic advection scheme (DO–PPA) [18], which has been validated with a MC formulation [15]. The same spatial and angular discretizations used for the first problem are found sufficient.

Transmittances from the frequency-dependent approach are presented in Fig. 5. As for the first problem, results from the space–frequency method are in good agreement with those from the literature [18]. It can also be seen that the physics of the problem is respected, since the transmittance begins exactly at $t^* = 1$.

A comparison between the frequency and time-dependent methods (exponential scheme [22], Van Leer flux limiter [23], and Superbee flux limiter [23]), at early time periods, is shown for this particular problem (Fig. 6). The minimal dimensionless time needed by the radiation to leave the slab of unit optical thickness is $t_L^* = 1$. Complete results are available in Ref. [24].

As for the first problem, results from the space–frequency method are the most accurate; the physics of the problem is respected, since the transmittance begins exactly at $t^* = 1$.

At the opposite of what have been observed for the first problem (Fig. 4), Fig. 6 does not report a significant difference between

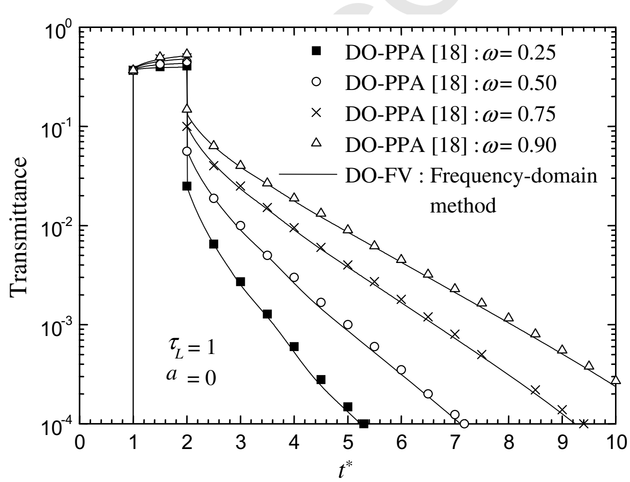

Fig. 5. Temporal distribution of hemispherical transmittance; comparison between the frequency domain approach and the DO–PPA method [18].

Table 2
CPU times associated with different time-based approaches and the frequency-based methods for problem 2

Resolution methods	CPU time (s)	Relative CPU time (Superbee flux limiter) [–]
Time domain approach, exponential scheme	143	0.57
Time domain approach, Van Leer flux limiter	225	0.89
Time domain approach, Superbee flux limiter	252	1
Frequency domain approach	1303	5.17

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the two approaches after t_L^*. This can be explained by the fact that, for a medium of unit optical thickness, the ballistic regime (collimated component) is dominant compared to the sinuous propagation regime (diffuse component), in the beginning of the temporal process. The collimated intensity does not induced early transmitted radiation, since its solution is determined exactly by a spatial exponential decay.

The CPU times associated with the different solution approaches are presented in Table 2, when the scattering albedo is 0.9. Previous conclusions hold.

5. Conclusion

The one-dimensional transient radiative transfer problem for absorbing and scattering media has been solved, in Cartesian coordinates, using a DO–FV approach based on the frequency domain.

It has been shown that the temporal distributions of transmittance obtained from the frequency domain approach are accurate, without the physically unrealistic fluxes emerging earlier than the minimal time required by the radiation to leave the medium.

However, compared to a time-dependent approach, the space–frequency method is time consuming (requires approximately, for all simulations carried out, five times more CPU time than solving directly the TRTE with a Superbee flux limiter). This can be explained by the fact that a large number of frequencies are needed to correctly represent the square pulse, and also, by the fact that the shift from the space–frequency to the space–time domain constitutes a supplementary computational step compared to a time-based technique.

A Fast FT algorithm was implemented to accelerate the IFT step, but the success of this strategy was mitig[illegible] no significant improvement in CPU time was reported [32]. The reason is that the IFT itself is not what burdens the algorithms, and the large CPU time are mostly due to the large numbers of angular frequencies. Therefore, a more physically realistic Gaussian incident pulse should be taken into account, since less angular frequencies would be required to adequately represent this temporal pulse.

6. Uncited reference

Q1 [11].

Acknowledgements

The author acknowledges Rodolphe Vaillon (CNRS researcher, CETHIL, INSA de Lyon) for his collaboration during these research works. But mostly, the author acknowledges Mathieu Francoeur (Graduate student, University of Kentucky) who did most of the work related to this paper. The author is also grateful to the Natural Sciences and Engineering Research Council of Canada (NSERC) for a discovery grant.

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