Numerical predictions of short-pulsed laser transport in absorbing and scattering media. I – A time-based approach with flux limiters.

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A one-dimensional transient radiative transfer problem in the Cartesian coordinate system involving an absorbing and scattering medium illuminated by a short laser pulse has computationally been solved by use of a Finite Volume Method (FVM). Previous works have shown that first order spatial interpolation schemes can not represent the physics of the problem adequately as transmitted fluxes emerge before the minimal physical time required to leave the medium. In this paper, the Van Leer and Superbee flux limiters, combined with the second order Lax-Wendroff scheme, are used in an attempt to prevent this. Results presented in this work show that despite significant improvement, flux limiters fail to completely eliminate the physically unrealistic behavior. Therefore, a numerical approach into which temporal variables are transformed into frequency-dependent variables is presented in the companion paper [1] to this work.

Keywords: radiative transfer; transient regime; short laser pulse; flux limiters; finite volume method

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NOMENCLATURE

a	asymmetry factor of the linear scattering phase function, -
c	speed of electromagnetic wave, $\mathrm{ms^{-1}}$
C_0	Courant number, -
H	Heaviside function, -
I	intensity, $\mathrm{Wm^{-2}sr^{-1}\mu m^{-1}}$
j	spatial node, -
m	discrete direction, -
n	temporal step, -
r	ratio of interpolation slopes, -
S_c	source function due to the scattering of the collimated component of intensity, $\mathrm{Wm^{-2}\mu m^{-1}}$
t	time, s
t^*	dimensionless time, -
T	hemispherical transmittance, -
w_m	angular weight, solid angle, -
z_L	thickness of the medium, m

Greek letters

β	extinction coefficient, $\mathrm{m^{-1}}$
Δ_+	slopes between intensities at nodes j and $j + 1$

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Δ_- slopes between intensities at nodes $j - 1$ and j

θ polar angle, rad

μ direction cosine relative to the polar angle, -

τ optical depth, -

τ_L optical thickness, -

ϕ azimuthal angle, rad

Φ scattering phase function, -

Ψ flux limiter, -

ω albedo for single scattering, -

Subscripts/Superscripts

$'$ other directions

0 incident collimated beam

c collimated component

d diffuse component

j refers to a spatial node

$j \pm ½$ refers to the boundaries of a control volume

L refers to medium thickness

m refers to a discrete direction

n refers to a temporal step

p refers to the pulse

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1. INTRODUCTION

Since the original work of Rackmil and Buckius [1], interest for transient radiative transfer has recently increased, mainly because of numerous possible uses of short pulse lasers in a wide variety of engineering and biomedical applications [2]. Optical diagnosis of absorbing and scattering media using temporal distributions of transmittance and/or reflectance remains a promising application of transient radiative transfer [2,3].

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 required by the radiation to leave the medium [2].

A wide variety of computational methods have been developed in order to solve the Transient Radiative Transfer Equation (TRTE), which describes the spatial and temporal variations of the radiation intensity into a participating medium along a particular direction. Among these methods: the Monte Carlo formulations [4,5], the classical Spherical Harmonics [2], the modified $MP_{1/3}A$ [6], the two-flux approaches [2], the Radiation Element Methods [7], the Discrete Ordinates approaches [8-10], the

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integral formulations [11,12] and, more recently, a backward method of characteristics [13,14].

In this paper, a Finite Volume Method (FVM) is proposed in the context of a one-dimensional problem. The reasons underlying this choice can be summarized as follows: (1) it makes use of an appropriate representation of the angular dependence of the radiation intensity (unlike a two-flux method), (2) it allows simplicity of implementation and solution (unlike high order Spherical Harmonics), (3) it involves relatively short computational times for convergence (unlike Monte Carlo formulations), and (4) it broadens the possibilities of angular discretization (unlike discrete ordinates methods).

Preliminary results [15] obtained with the FVM embedding first order spatial interpolation schemes (upwind and exponential), have shown that the model induces transmitted radiative fluxes that emerge earlier than the minimal time required by the radiation to leave the medium. This unphysical result has been reported elsewhere in the literature [8-10] and constitutes the main drawback of the FVM and other methods applied to the solution of 1-D transient radiative transfer. This is caused mainly by the interdependence between the spatial and temporal discretizations, and the numerical approximations embedded within the application of an interpolation scheme. Here, the main objective of this paper is to minimize the unphysical results associated with the propagation of a sharp wave front. This is done by the implementation of a second order interpolation scheme (Lax-Wendroff) coupled with flux limiters into the FVM as some researchers [8,9,16,17] have proposed similar ideas in attempts to overcome the problem.

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The theoretical formulation is summarized in the second section: the problem is described, the assumptions are formulated, and the TRTE is presented. The FVM formulation along with the application of the Van Leer and Superbee flux limiters are afterwards the subject matter of section 3. The proposed method is then applied to two typical 1D transient radiative transfer problems, and results are compared with those obtained with a first order exponential scheme [15] and with those available in the literature. Concluding remarks are presented in the fifth section of the paper.

2. THEORETICAL FORMULATION

2.1. Transient radiative transfer 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 refractive index of unity; (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; (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, i.e. the pulse width is less than the characteristic time for the establishment of any other

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phenomenon [2]. This typical one-dimensional transient radiative transfer problem is schematically depicted in figure 1.

[Insert figure 1 about here]

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 of 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 metrological applications [2,3,18]. A similar conclusion holds with respect to temporal distributions of the reflectance.

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2.2. Mathematical modeling

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 [19]. 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 [8].

The TRTE describes spatial and temporal variations of the diffuse component of the intensity along the direction μ in the absorbing and scattering medium. Using dimensionless time ($t^* = \beta ct$) and optical depth ($\tau = \beta z$) as variables, the one dimensional TRTE is written as follows [19]:

$$\frac{\partial I_d(\tau,\mu,t^*)}{\partial t^*} + \mu \frac{\partial I_d(\tau,\mu,t^*)}{\partial \tau} =$$

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

The first and second terms on the right-hand side of equation (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 [8,15] :

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

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

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

3. NUMERICAL SOLUTION

3.1. Finite Volume formulation

The radiation intensity, following the assumptions stated in the previous section, is space, direction, and time dependent. As analytical solutions are few, it is therefore necessary to discretize these three independent variables in order to solve the TRTE computationally.

In a one-dimensional Finite Volume approach in Cartesian coordinates, the spatial domain is discretized in J non-overlapping control volumes $\Delta\tau_j$. The method implemented here also involves a discretized angular domain into M directions of equal angular weight w_m [19]. This uniform angular discretization respects the half-range first moment as well as the full-range zeroth moment to fulfill this need for energy conservation [20]. Finally, the temporal variations of the TRTE are approximated by defining N finite time steps Δt_n^*.

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Then, integrating the TRTE over a control space $\Delta\tau_j w_m \Delta t_n^*$ with a temporal implicit scheme yields [15]:

$$I_j^{m,n} = \frac{\dfrac{1}{\Delta t_n^*} I_j^{m,n-1} - \dfrac{\mu_m}{\Delta\tau_j}\left(I_{j+1/2}^{m,n} - I_{j-1/2}^{m,n}\right) + \dfrac{\omega_j}{2}\sum_{m'=1}^{M} w_{m'} I_j^{m',n} \Phi_j^{m'm} + S_{c_j}^{m,n}}{\dfrac{1}{\Delta t_n^*} + 1} \tag{4}$$

In the above, $I_j^{m,n}$ is the intensity at node *j*, in direction *m*, and at time step *n*, while $I_{j\pm1/2}^{m,n}$ are the intensities at the boundaries of the control volume. The subscript *d*, referring to the diffuse component of the intensity, is omitted for clarity.

To solve equation (4), one needs to relate the value of the intensity at a node (…, *j* – 1, *j*, *j* + 1,…) – for a specific direction and time step – to the value of the intensity at control volume faces (*j* ± ½), provided that here a prevailing assumption is implicitly involved for both the value of intensity over a control solid angle w_m and over a control time step Δt_n^*.

When an appropriate spatial interpolation scheme is selected, equation (4) is then solved for each node *j*, in each direction *m*, and for each time step *n* of the spatial, angular, and temporal 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.

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3.2. Flux limiters

A moving pulsed collimated radiation beam in an absorbing and scattering medium is schematically depicted in figure 2. This figure can be seen as a snapshot of the wave front of the pulse at a particular instant t_n^*.

[Insert figure 2 about here]

As described in figure 2 at instant t_n^*, the front of the pulse is located at position τ_j (node j). Consequently, from a theoretical point of view, intensities located within the range of the front of the pulse ($\tau \leq \tau_j$) are necessarily greater than zero, while intensities located beyond this front ($\tau > \tau_j$) are equal to zero. However, from a numerical point of view, intensities at nodes $j + 1$, $j + 2$, …, J could be non-zero due to the numerical approximations embedded in the interpolation scheme. This temporal numerical diffusion would then lead to the aforementioned error, that is radiative fluxes emerging earlier than the minimal time required by the radiation to leave the medium. A FVM coupled with first order spatial interpolation schemes leads to such unrealistic results [15]. These early transmitted radiative fluxes can be partially minimized by applying the Courant stability criteria expressed here as: $\Delta t_n^* < \min\{\Delta\tau_j\}$ [15,21]. This condition simply ensures that for a given temporal step, the wave front of the pulse can not propagate within more than one control volume at a time. Here, the Courant number C_0 has been defined as

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$\Delta t_n^*/\min\{\Delta\tau_j\}$. Therefore, the temporal numerical diffusion decreases with decreasing Courant numbers.

However, this has been found to be insufficient and the second order spatial interpolation Lax-Wendroff (L-W) scheme, originally proposed for Eulerian transport problems in hydrodynamics, is used in this work [21]. This scheme, based on the decomposition of the dependent variable (radiation intensity) into Taylor series expansion truncated after the second order term, implies (for $\mu > 0$) [21]:

$$I_{j+1/2}^{m,n} = I_j^{m,n} + \frac{1}{2}(1 - \Delta t_n^* / \Delta\tau_j)(I_j^{m,n} - I_{j-1}^{m,n}) \quad (5)$$

Equation (5) stipulates that the intensity at the boundary $j + 1/2$ of the control volume is computed with a linear interpolation (figure 3), where the slopes are represented by Δ_+ (between nodes j and $j+1$) and Δ_- (between nodes $j - 1$ and j).

[Insert figure 3 about here]

This numerical approach has been found to reduce the temporal numerical diffusion, but introduces, in counterpart, significant oscillations near the discontinuity (i.e., at the front of the pulse) [21]. In that case, a correction factor must be introduced in order to ensure a monotonicity preserving scheme [8,17,19,22]. Such a monotonicity preserving scheme ensures that when the initial distribution of a moving quantity is monotonic, the resulting distribution is also monotonic. In other words, this condition prevents the creation of false extremas, or a false amplification of existing extremas (i.e. eliminates the oscillations).

The introduction of a flux limiter Ψ_j in equation (5) enables one to keep the solution monotonic and allows the accuracy of a second order spatial interpolation scheme. The L-W scheme is consequently modified such that (for $\mu > 0$) [17,21]:

$$I_{j+1/2}^{m,n} = I_j^{m,n} + \frac{1}{2}\Psi_j (1 - \Delta t_n^* / \Delta\tau_j)(I_j^{m,n} - I_{j-1}^{m,n}) \tag{6}$$

The value of Ψ_j must be determined by the spatial distribution of intensity; this is done by the introduction of the variable r_j [17]:

$$r_j = \frac{I_{j+1}^{m,n} - I_j^{m,n}}{I_j^{m,n} - I_{j-1}^{m,n}} \tag{7}$$

The right-hand side of equation (7) simply represents the ratio of the slopes Δ_+ and Δ_- in the particular case of a regular spatial discretization (see figure 3). In this work, the Van Leer flux limiter is used, and is written as [17,21]:

$$\Psi_j = \frac{r_j + |r_j|}{1 + |r_j|} \tag{8}$$

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Equation (8) implies that when there is a discontinuity around node j (slopes Δ_+ and Δ_- of opposite signs), r_j takes a negative value and the flux limiter Ψ_j becomes equal to zero. Consequently, the interpolation scheme is akin to the upwind scheme. On the other hand (slopes Δ_+ and Δ_- of same signs), the interpolation slope at the node j is determined by the harmonic mean of the slopes Δ_+ and Δ_-.

Another flux limiter, called Superbee, is used in this paper, and is defined as [17,21]:

$$\Psi_j = \max[0, \min(1, 2r_j), \min(r_j, 2)]. \tag{9}$$

In this case, the value of Ψ_j is determined by comparing the slopes Δ_+ and Δ_- around node j. As for the Van Leer flux limiter, Ψ_j equals zero when the slopes Δ_+ and Δ_- are of opposite signs. It is important to note that numerical details regarding flux limiters are beyond the scope of this paper, and are available elsewhere [21].

4. NUMERICAL RESULTS

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 at $\tau = 0$ (figure 1). When the medium is anisotropically scattering, the linear anisotropic phase function is considered ($\Phi(\mu,\mu') = 1 + a\mu\mu'$) [19].

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The numerical implementations of the proposed formulation are written in *FORTRAN* and originally compiled with *Microsoft Developer Studio – Fortran PowerStation 4* on a single processor desktop PC.

4.1. Problem 1: Optically thick and highly scattering medium

In this first problem, the optical thickness of the medium is τ_L = 10 while the scattering albedo is ω = 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 [22]) are sufficient to discretize the spatial and directional domains; no significant improvement of the results has been observed beyond these thresholds. The temporal discretization is determined by analyzing the Courant number defined in section 3.2; numerical simulations have been performed, and a Courant number of 0.2 has been found to be optimal (results not presented).

Transmittances obtained from the DO-FV and the Van Leer flux limiters are presented in figure 4, and compared with those obtained from a Monte Carlo (MC) formulation for the same problem [5]. It is important to note that since the optical thickness of the slab is 10, the minimal dimensionless time required by the radiation to leave the medium is also 10.

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[Insert figure 4 about here]

The sharp diminution of transmittance at t^* = 11, followed by an increase, is due to 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.

Figure 4 clearly indicates that for a large time scale (from 0 to 100), results obtained with the Van Leer flux limiter are in good agreement with those obtained with a reference Monte Carlo approach, even at early time periods. The same conclusion is applicable for the Superbee flux limiter, as shown in figure 5.

[Insert figure 5 about here]

In order to analyze more precisely the relative accuracy of flux limiters, the transmittances are compared at early time periods with results obtained with a first order exponential scheme [15]. Only results for a = 0.9 are shown, since early transmitted radiation becomes more important as the medium is highly forward scattering.

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[Insert figure 6 about here]

Figure 6 shows that the radiative flux leaving the medium before the minimal physical dimensionless travel time t_L^* = 10 is considerably decreased with the flux limiters. Generally, for all simulations carried out prior to this paper, the Superbee flux limiter lead to more accurate results than the Van Leer. Despite this fact, early transmitted radiation can not be completely avoided.

4.2. Problem 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 solved with a Discrete Ordinates approach coupled with the Piecewise Parabolic Advection scheme (DO-PPA) [8], which has been validated with a Monte Carlo formulation [5]. The same spatial, angular, and temporal discretizations used for the first problem are found sufficient.

The transmittances, obtained from the DO-FV method coupled with the Van Leer and Superbee flux limiters, are presented in figures 7 and 8, respectively. In this case, the minimal dimensionless time needed by the radiation to leave the slab of unit optical thickness is t_L^* = 1.

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[Insert figure 7 about here]

[Insert figure 8 about here]

The transmittance is more important as the scattering albedo increases. This can be explained by the fact that a larger proportion of the pulsed collimated radiation beam is scattered in the medium. Moreover, an increase of the scattering albedo leads to a diminution of the mean free path of scattering, and hence to an increase of multiple scattering, longer photons travel paths, and, consequently, a larger transmitted temporal signal. Here again, the decrease of transmittance at $t^* = 2$ is due to the fact that the collimated component of radiation intensity has left the medium. After $t^* = 2$, the transmittance is only due to the diffuse part of radiation intensity.

It can be seen in figures 7 and 8 that the temporal distributions of transmittances are, in general, in good agreement with those obtained from the DO-PPA. However, early transmitted radiation can be observed on a temporal scale from 0 to 10, for both types of flux limiters.

Figure 9 shows a comparison between transmittances obtained with the first order exponential scheme [15] and flux limiters at early time periods for a scattering albedo of $\omega = 0.9$.

[Insert figure 9 about here]

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It is clear from figure 9 that the Superbee flux limiter leads to more accurate results, even if there is still radiation transmitted before $t^* = 1$.

5. CONCLUSION

The one-dimensional transient radiative transfer problem for absorbing and scattering media has been solved in Cartesian coordinates using a Discrete Ordinates – Finite Volume approach. The Van Leer and Superbee flux limiters, based on the second order spatial scheme Lax-Wendroff, have been used in order to minimize the transmitted fluxes emerging before the minimal time required by the radiation to leave the medium.

In general, results from the DO-FV coupled with flux limiters are in close agreement with those from the literature. Moreover, a comparison at early time periods with the transmittance obtained from a DO-FV and a first order exponential scheme has shown that the flux limiters can substantially decrease the temporal numerical diffusion. However, there is still a low transmitted flux before the minimal physical time required by the radiation to leave the medium.

High order schemes coupled with flux limiters can not totally avoid this problem. Indeed, a DO-FV formulation based in the space-time domain will never completely prevent this problem due to the interdependence between the spatial and temporal discretizations.

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Therefore, second part of this work is devoted to the formulation, implementation, and validation of a method for which the transient radiative transfer problem is solved in the space-frequency domain.

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FIGURES

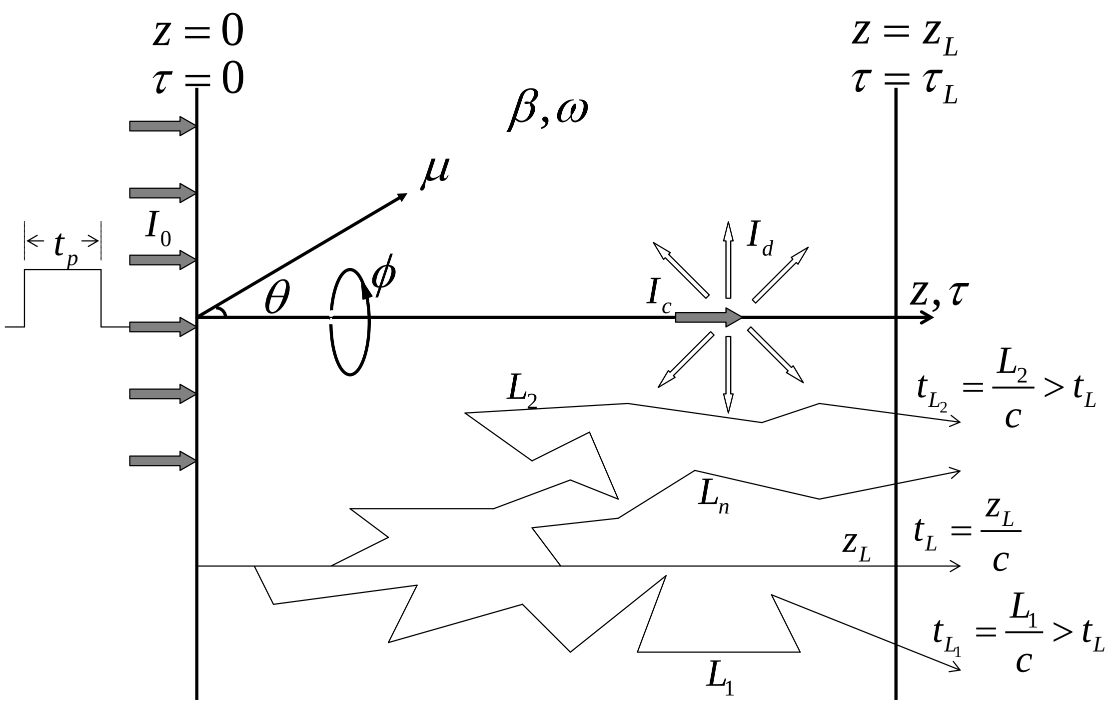

Figure 1: Schematic representation of the transient radiative transfer problem under consideration.

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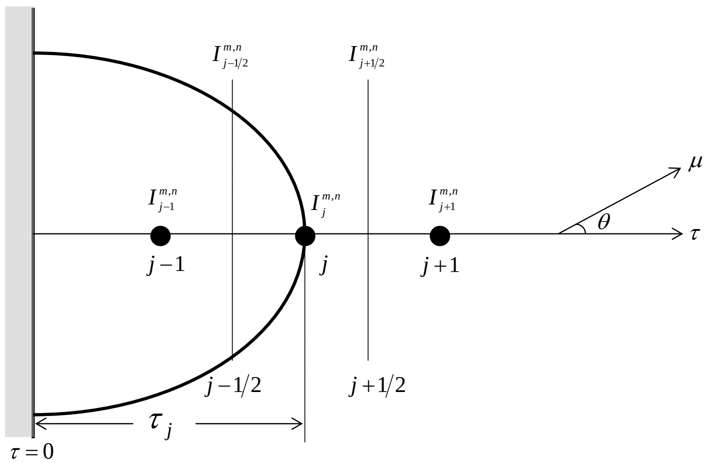

Figure 2: Schematic representation of a pulsed collimated radiation beam propagating in a participating medium.

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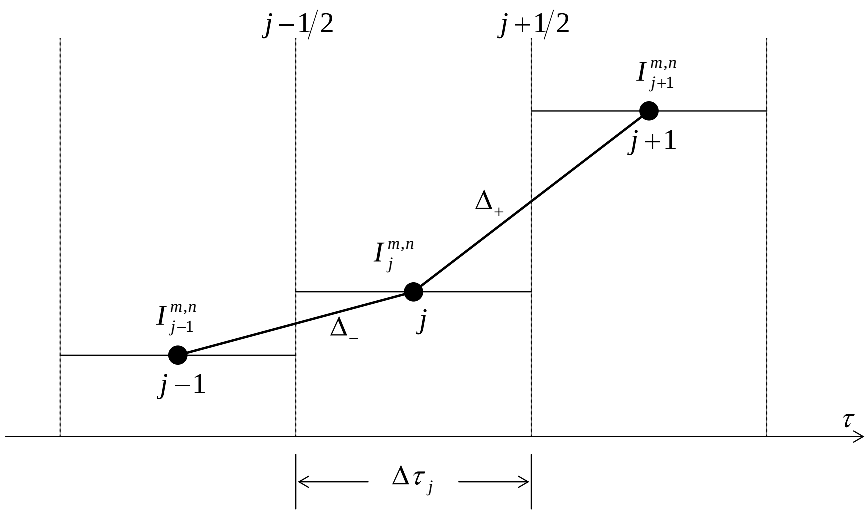

Figure 3: Representation of a control volume and its surrounding nodes.

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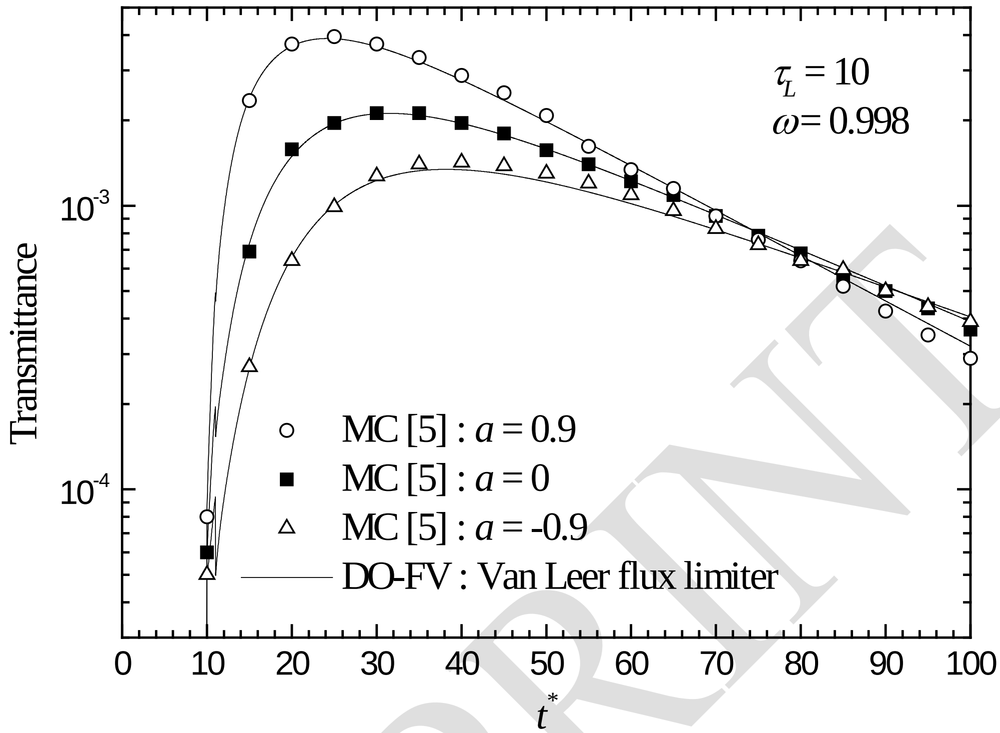

Figure 4: Temporal distribution of the hemispherical transmittance; comparison between the Van Leer flux limiter and a Monte Carlo formulation [5].

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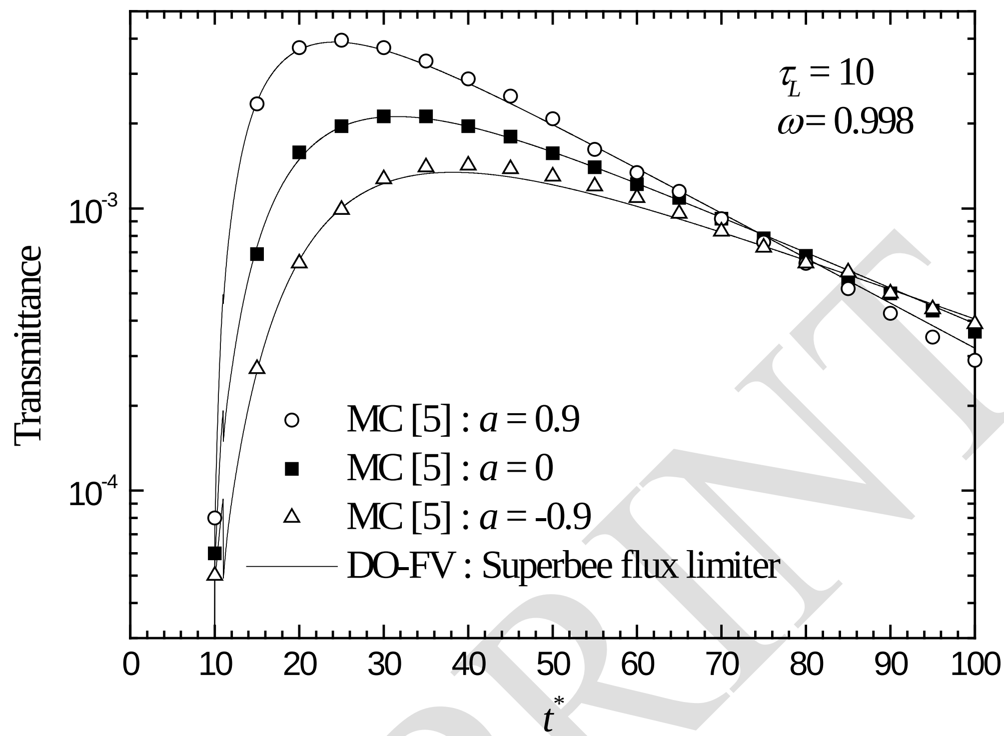

Figure 5: Temporal distribution of the hemispherical transmittance; comparison between the Superbee flux limiter and a Monte Carlo formulation [5].

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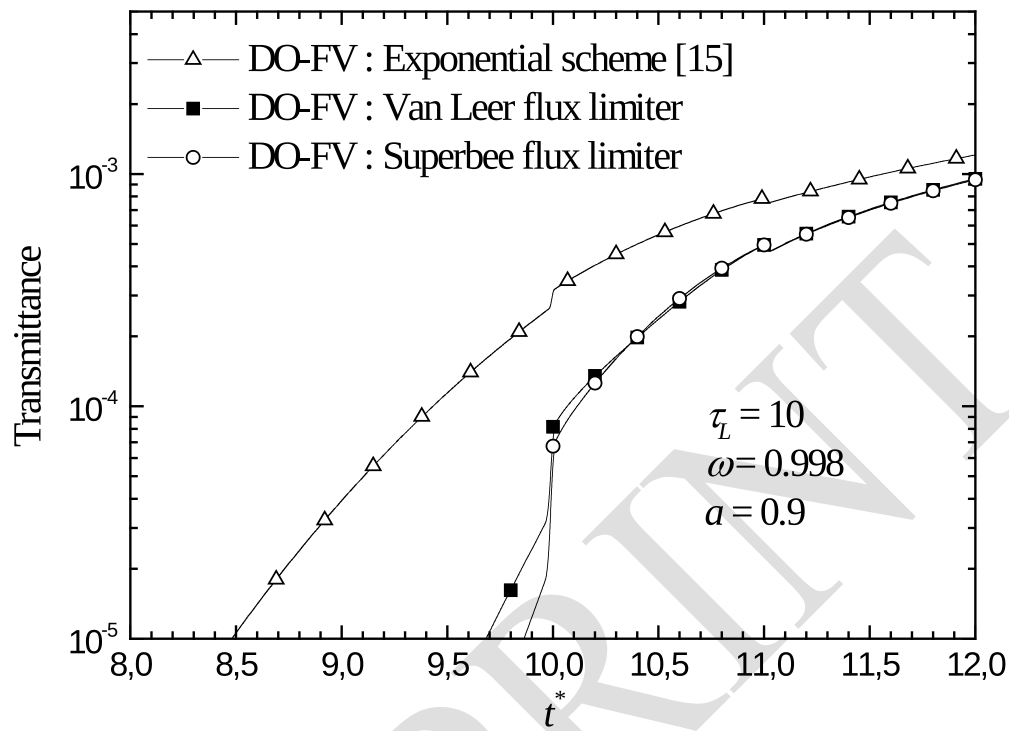

Figure 6: Temporal distribution of the hemispherical transmittance; comparison between the Van Leer and Superbee flux limiters and the exponential interpolation scheme at early time periods.

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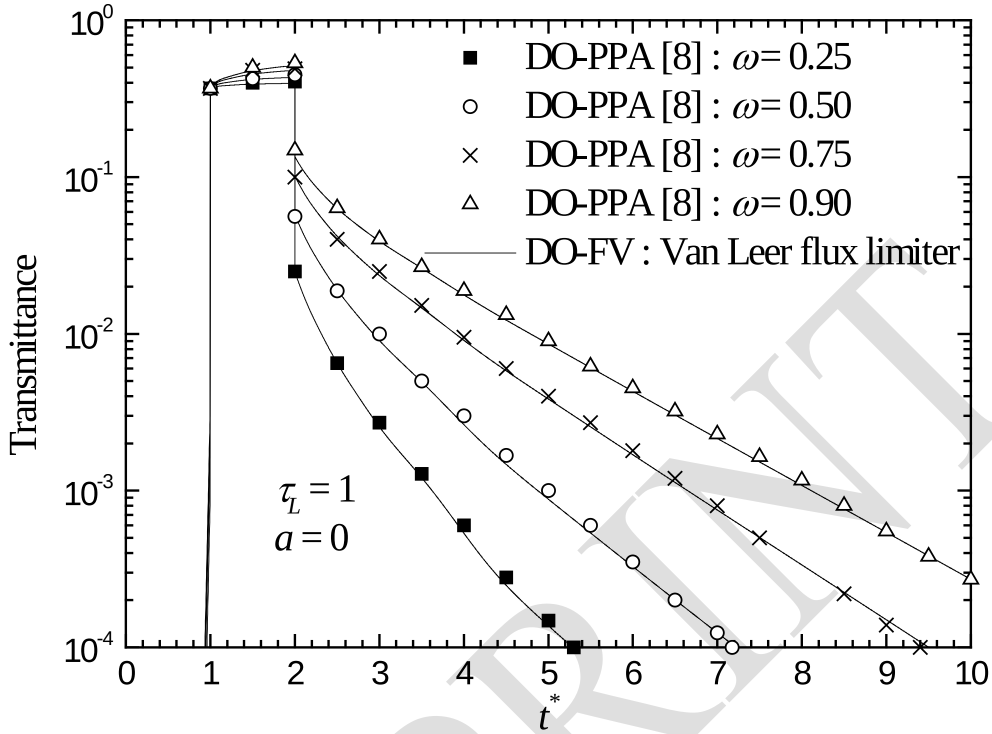

Figure 7: Temporal distribution of the hemispherical transmittance; comparison between the Van Leer flux limiter and the DO-PPA method [8].

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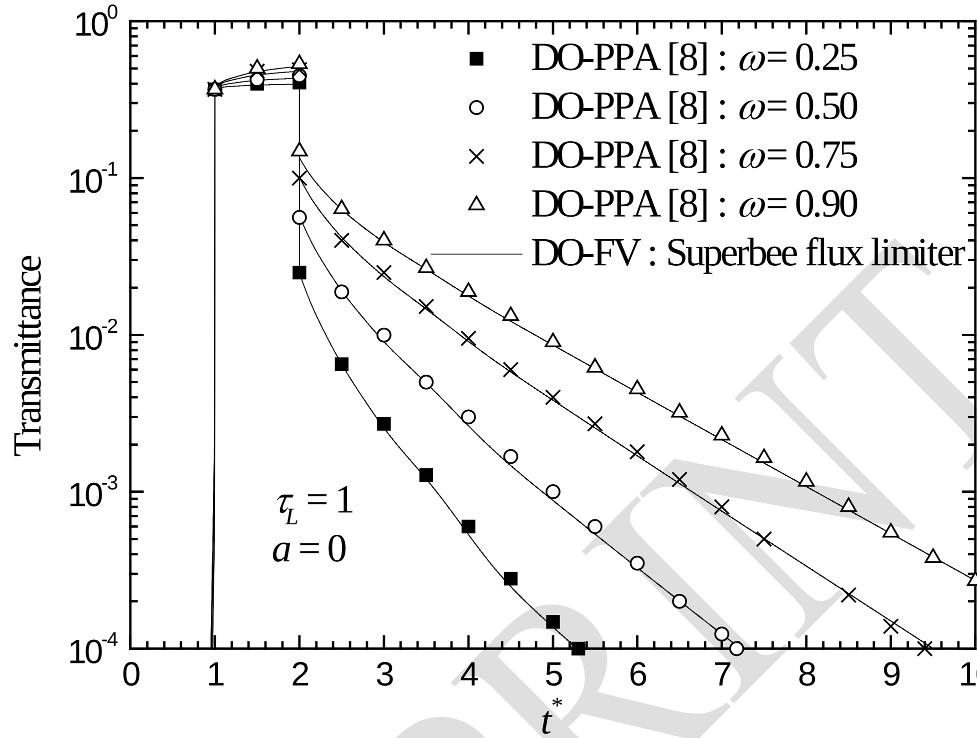

Figure 8: Temporal distribution of the hemispherical transmittance; comparison between the Superbee flux limiter and the DO-PPA method [8].

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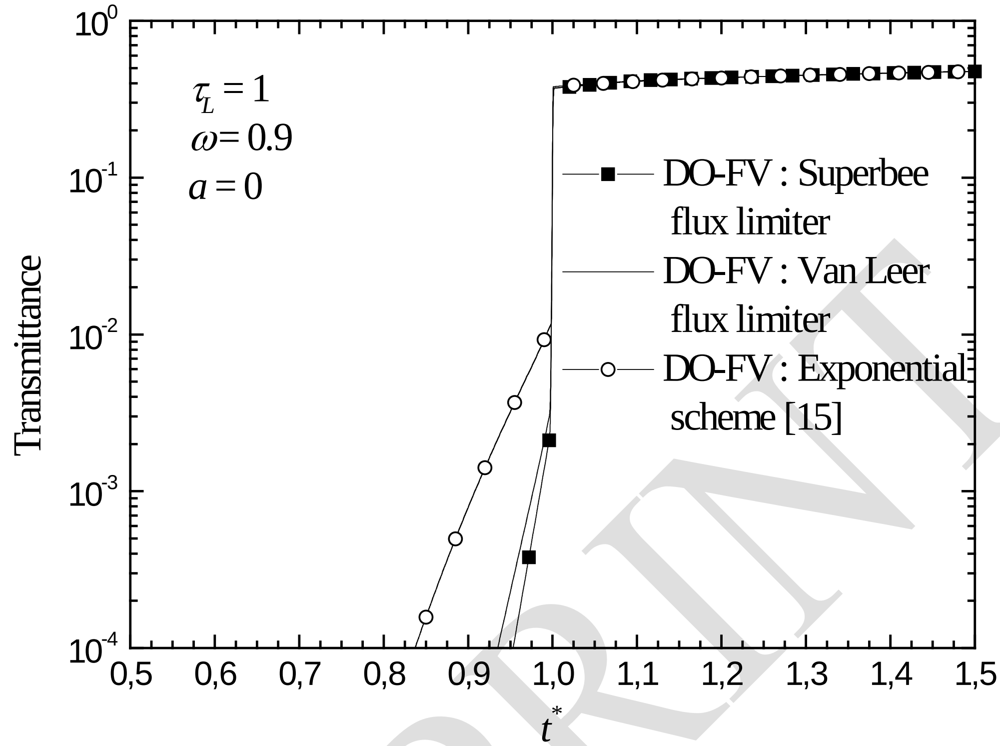

Figure 9: Temporal distribution of the hemispherical transmittance; comparison between the Van Leer and Superbee flux limiters and the exponential interpolation scheme at early time periods.

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