

A Random Walk Method for Solving Radiative Transfer Equations

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One approximates Fleck's radiative transfer equation by a diffusion equation when the mean free path of the photons is small. This diffusion approximation is used in a Monte Carlo method to substitute a jump of the particles for a large number of collisions in the optically thick media. © 1987 Academic Press, Inc.

INTRODUCTION

To solve numerically the radiative transfer equations on a fixed time step, Fleck and Cummings [1] have proposed to evaluate implicitly the emission temperature through a linearization of the energy balance equation.

Therefore in the photon transfer equation, we substitute a pseudo-scattering term for a part of the emission-absorption terms. With this time discretisation scheme, the radiative intensity $I(t, \mathbf{x}, \boldsymbol{\Omega}, \nu)$ of the photons (at time t , position \mathbf{x} , with the direction $\boldsymbol{\Omega}$ and the frequency ν) satisfy the so-called Fleck's equation on each time step

$$\begin{aligned} \frac{1}{c} \frac{\partial I}{\partial t} + \boldsymbol{\Omega} \cdot \frac{\partial I}{\partial \mathbf{x}} + k_a I + k_{Th} Q I \\ = k_a b l \phi + k_a b (1-l) \frac{\int_0^\infty \int_{S^2} k_a(\nu') I(\boldsymbol{\Omega}', \nu') (d\boldsymbol{\Omega}'/4\pi) d\nu'}{\int_0^\infty k_a(\nu') b(\nu') d\nu'} \end{aligned} \quad (*)$$

where: \mathbf{x} belongs to a spatial domain D of \mathbb{R}^3 , $\boldsymbol{\Omega}$ belongs to the unit sphere S^2 of \mathbb{R}^3 , and ν belongs to $(0, \infty)$. The temperature T is assumed to be constant on each spatial cell. For this temperature, denote by $b(\nu)$ the reduced Planck function, by $k_a(\nu)$ the absorption coefficient and by l Fleck's coefficient. Moreover ϕ is equal to T^4 , up to a constant.

Q is the Thomson scattering operator which corresponds to the changing of the direction of the photon velocity.

The classical Monte Carlo method is well adapted to solve Fleck's equation (*) if the pseudo scattering mean free path $[(1-l)k_a]^{-1}$ is not too small with respect to the size of D , that is, if the scattering term is less important than the streaming terms. But in an optically thick medium $(1-l)$ is very close to 1 and k_a is very

large, thus the pseudo-scattering mean free path is very small and there are a lot of collisions in any small subdomain; so the tracking of the particle becomes highly time consuming.

To accelerate this Monte Carlo method, we describe in this paper a method to avoid very complex trackings of the particles in the optically thick media. The principle of this method is to use a jump as a substitute for the trajectory of a particle which undergoes a large number of collisions in a cell. This jump will be sampled according to the law $\bar{I}(t, \cdot)$, where \bar{I} is the solution of a diffusion equation which approximates (*) in the case of an opaque medium.

In order to find this approximation we make an appropriate scaling in equation (*) with a small parameter ε related to the mean free path $k_a(v)^{-1}$ of the particles and we calculate the limit \bar{I} of the solution I of (*) when ε goes to 0 (this is the multiple scale technique).

We first give the result of the calculation with an error of order $O(\varepsilon^2)$ (in Sect. 2.1) and an improvement of this result is given in Section 2.2. This method works because the limit equation is simple enough and it is easy to have an explicit solution of this equation, if we consider the case where the spatial cell is a sphere D .

In Section 3 we derive the transfer equation satisfied by a Monte Carlo particle and we give the explicit solution of the corresponding diffusion equation. This solution gives the law of the escape time of the particle out of the sphere D and the space distribution law of the particle at the end of the time step if it has not escaped. Afterwards (Sect. 4) we study some criteria for the validity of the diffusion approximation using a Monte Carlo computation in a sphere. Numerical results are given in the last section, they show that there is a very good agreement between the classical Monte Carlo method and the method which is accelerated by the random walk procedure, although the computer time is much shorter.

From a philosophical point of view, this method looks like the one of Fleck and Canfield [2] and Lynch [3]. But the way to determine the characteristics of the jump replacing the tracking of the particle is based on an analytic method instead of a probabilistic one; then it is possible to determine when it is appropriate to substitute a "random walk" jump for the detailed tracking of the particles.

The outline of this paper is:

1. *Setting of the problem.*
2. *Approximation results.* • First result. • Improvement of the approximation.
3. *Diffusion approximation of the transport equation satisfied by a Monte Carlo particle.* • The transport equation for a particle. • The diffusion approximation. • Explicit solution of the diffusion equation.
4. *The random walk procedure.* • Criteria for random walk. • Description of the random walk procedure.
5. *Numerical results. References.*

1. SETTING OF THE PROBLEM

We consider the radiative transfer phenomena during only one time step (say: $[0, t^1]$ for the sake of simplicity). The framework of Fleck's modelization is the following one (see Fleck-Cummings [1]).

The absorption coefficient is assumed to be independent of time and space variables in D and the initial temperature T is assumed to be constant on D .

Let us denote

- c , the velocity of light,
- Φ , the material temperature to the 4th power up to the multiplicative constant $ac/4\pi$ ($ac/4$ is Stephan's constant): $\Phi = (ac/4\pi) T^4$, and

$$b(\nu) = \frac{15}{\pi^4} \frac{\xi^3}{e^\xi - 1} \frac{h}{KT} \quad \left(\xi = \frac{h\nu}{KT} \text{ and } h, K \text{ are classical constants} \right);$$

that is, $\int_0^\infty b(\nu) d\nu = 1$; $\Phi b(\nu)$ is the Planck function.

- $k_{Th}(\nu)$, Thomson's scattering coefficient,
- $k_a(\nu)$, the absorption coefficient,
- $k_P = \int_0^\infty k_a(\nu) b(\nu) d\nu$, Planck's absorption coefficient,
- $\mathcal{E}(\Phi)$, the specific internal energy; $\mathcal{E}' = \partial \mathcal{E} / \partial \Phi$.
- $l = [1 + 4\pi c t^1 \mathcal{E}'^{-1} k_P]^{-1}$, Fleck's coefficient, (1)
- $\sigma_a(\nu) = lk_a(\nu)$, pseudo-absorption coefficient, (2)
- $\sigma_s(\nu) = (1 - l) k_a(\nu)$, pseudo-scattering coefficient. (3)

Then the radiative intensity $I = I(t, \mathbf{x}, \Omega, \nu)$ satisfies

$$(i) \quad \frac{1}{c} \frac{\partial I}{\partial t} + \mathbf{\Omega} \frac{\partial I}{\partial \mathbf{x}} + (\sigma_a + \sigma_s) I + k_{Th} QI - \frac{h_a b}{h_p} \int_0^\infty \int_{S^2} \sigma_s(\nu') I(\mathbf{\Omega}', \nu') \frac{d\mathbf{\Omega}'}{4\pi} d\nu' = \sigma_a b \Phi \tag{4}$$

$$(ii) \quad I(t, \mathbf{x}, \mathbf{\Omega}, \nu) = 0, \quad \text{on } \partial D^-$$

$$(iii) \quad I(0, \mathbf{x}, \mathbf{\Omega}, \nu) = I^{in}(\mathbf{x}, \mathbf{\Omega}, \nu),$$

where $\partial D^- = \{ \mathbf{x} \in \partial D, \mathbf{\Omega} \in S^2 / \mathbf{n}_x \cdot \mathbf{\Omega} \leq 0 \}$, \mathbf{n}_x is the outward unit normal at \mathbf{x} to the boundary ∂D , and Q is the Thomson scattering operator defined by

$$(QI)(\mathbf{x}, \mathbf{\Omega}, \nu) = I(\mathbf{x}, \mathbf{\Omega}, \nu) - \int_{S^2} [1 + (\mathbf{\Omega}\mathbf{\Omega}')^2] \frac{3}{4} I(\mathbf{\Omega}') \frac{d\mathbf{\Omega}'}{4\pi}$$

$I^{in} = I^{in}(\mathbf{x}, \mathbf{\Omega}, \nu)$ is the initial radiative intensity.

Then we have to solve the following scalar equation in order to find the temperature Φ^1 at time t^1 ,

$$\mathcal{E}(\Phi^1) - \mathcal{E}(\Phi) = E_{\text{abs}}/|D| - 4\pi t^1 k_p \Phi,$$

where E_{abs} is the absorbed energy in $D \times [0, t^1]$,

$$E_{\text{abs}} = \int_0^{t^1} dt \int_D d\mathbf{x} \int_0^\infty dv \int_{S^2} d\Omega \sigma_a(v) I(t, \mathbf{x}, \Omega, v)$$

and $|D|$ is the volume of D .

2. APPROXIMATION RESULTS

In an opaque cell the mean free path between two collisions becomes very small, the frequency distribution of the particles converges towards a Planck function, the velocity distribution becomes isotropic, and the spatial density becomes very close to the density of a diffusion process. The aim of this section is to give a mathematical form of this fact.

Therefore consider an opaque cell D and assume that

$$\sigma_s^{-1} \text{ is small enough with respect to the characteristic size of } D, \quad (6)$$

$$l \text{ is small enough with respect to } 1. \quad (7)$$

So we introduce a small parameter ε and define

$$\begin{aligned} \sigma(v) &= \varepsilon \sigma_s(v) \\ q(v) &= \frac{1}{\varepsilon} \sigma_a(v) \\ \omega &= \varepsilon k_{\text{Th}} \\ \hat{t} &= \varepsilon ct. \end{aligned} \quad (8)$$

Let us introduce some notation:

$\bar{\mathbf{x}}$ is the projection of a point \mathbf{x} of D onto ∂D

$$\begin{aligned} \langle\langle f \rangle\rangle &= \int_0^\infty \int_{S^2} f(\Omega', v') \frac{d\Omega'}{4\pi} dv'; \\ \sigma_p &= \langle\langle \sigma b \rangle\rangle; \quad q_p = \langle\langle qb \rangle\rangle \quad [\text{then } \varepsilon^2 q_p \sigma_p^{-1} = l(1-l)^{-1}]; \\ Lf &= \sigma f - \sigma_p^{-1} \sigma b \langle\langle \sigma f \rangle\rangle + \omega Qf; \\ I_\varepsilon(\hat{t}, \mathbf{x}, \Omega, v) &= I(\hat{t}/\varepsilon c, \mathbf{x}, \Omega, v). \end{aligned} \quad (9)$$

Equation (4) may be written in the form

$$\begin{aligned}
 \text{(i)} \quad & \frac{\partial I_\varepsilon}{\partial \hat{t}} + \frac{1}{\varepsilon} \mathbf{\Omega} \cdot \frac{\partial I_\varepsilon}{\partial \mathbf{x}} + \frac{1}{\varepsilon^2} L I_\varepsilon + q I_\varepsilon = qb\Phi \\
 \text{(ii)} \quad & I_\varepsilon(\hat{t}, \cdot) = 0 \quad \text{on } \partial D^- \\
 \text{(iii)} \quad & I_\varepsilon(0, \cdot) = I^{in}.
 \end{aligned}
 \tag{10}$$

2.1. First Result

Let us denote the Laplace operator by Δ_x .

PROPOSITION 1. *Let I be the solution of (10). Let u_0 and u_1 be the solutions of the diffusion equations*

$$\begin{aligned}
 \text{(i)} \quad & \frac{\partial u_0}{\partial \hat{t}} - \frac{1}{3\sigma_0} \Delta_x u_0 + q_p(u_0 - \phi) = 0 \\
 \text{(ii)} \quad & u_0(\hat{t}, \mathbf{x}) = 0 \quad \text{on } \partial D \\
 \text{(iii)} \quad & u_0(0, \mathbf{x}) = \langle\langle I^{in}(\mathbf{x}) \rangle\rangle,
 \end{aligned}
 \tag{12}$$

$$\begin{aligned}
 \text{(i)} \quad & \frac{\partial u_1}{\partial \hat{t}} - \frac{1}{3\sigma_0} \Delta_x u_1 + q_p u_1 = 0 \\
 \text{(ii)} \quad & u_1(\hat{t}, \mathbf{x}) + \varepsilon \frac{L_0}{\sigma_0} \frac{\partial u_0}{\partial n}(\hat{t}, \mathbf{x}) = 0 \quad \text{on } \partial D \\
 \text{(iii)} \quad & u_1(0, \mathbf{x}) = 0
 \end{aligned}
 \tag{12'}$$

with $\sigma_0 = \langle\langle b/(\sigma + \omega) \rangle\rangle$ and where L_0 is a constant depending only on σ/σ_p and ω . Then there exist two functions $\varphi = \varphi(s; \mathbf{x}, \mathbf{\Omega}, v)$ and $\psi = \psi(\xi; \hat{t}, \bar{\mathbf{x}}, \mathbf{\Omega}, v)$ corresponding to an initial layer term and a boundary layer term [i.e., they satisfy

$$\lim_{s \rightarrow \infty} \varphi(s; \cdot) = 0, \quad \lim_{\xi \rightarrow \infty} \psi(\xi; \cdot) = 0],$$

and we have for small ε ,

$$\begin{aligned}
 & I_\varepsilon(\hat{t}, \mathbf{x}, \mathbf{\Omega}, v) - \left\{ b(v) u_0(\hat{t}, \mathbf{x}) + \varepsilon \left[b(v) u_1(\hat{t}, \mathbf{x}) - \mathbf{\Omega} \cdot \frac{b(v)}{\sigma(v) + \omega} \frac{\partial u_0}{\partial \mathbf{x}}(\hat{t}, \mathbf{x}) \right] \right. \\
 & \left. + \varphi\left(\frac{\hat{t}}{\varepsilon^2}; \mathbf{x}, \mathbf{\Omega}, v\right) + \varepsilon \psi\left(\frac{\xi_x}{\varepsilon}; \hat{t}, \bar{\mathbf{x}}, \mathbf{\Omega}, v\right) \right\} = O(\varepsilon^2),
 \end{aligned}
 \tag{12''}$$

where ξ_x is the distance between \mathbf{x} and ∂D ($\xi_x = (\bar{\mathbf{x}} - \mathbf{x}) \cdot \mathbf{n}_x$).

The meaning of this proposition is the following. In an opaque cell D , except in a short time near $\hat{t}=0$ and except in a boundary layer, the spectral distribution of the solution I_ε is a Planck distribution, and I_ε may be well approximated by

$$b(\nu) \left[u_0 + \varepsilon u_1 - \frac{\varepsilon}{\sigma(\nu)} \boldsymbol{\Omega} \cdot \frac{\partial u_0}{\partial \mathbf{x}} \right].$$

The details of the proof are given in Giorla-Sentis [4] but we give here the formal calculus which is behind this result, using the multiple scale technique. (This technique has been used for a long time in transport problems in a large number of papers including [5, 6] and the references of these papers.)

First, one considers the asymptotic expansion of I_ε ,

$$I_\varepsilon = I_0 + \varepsilon I_1 + \varepsilon^2 I_2 + \varepsilon^3 I_3 + \varphi \left(\frac{\hat{t}}{\varepsilon^2}; \mathbf{x}, \boldsymbol{\Omega}, \nu \right) + \varepsilon \psi \left(\frac{\xi}{\varepsilon}; \hat{t}, \bar{\mathbf{x}}, \boldsymbol{\Omega}, \nu \right) + I_{\text{rem}}.$$

One introduces this expansion in Eq. (10). When one sets to zero the terms which are of order ε^{-2} , ε^{-1} and ε^0 one obtains

$$L I_0 = 0 \quad (13.1)$$

$$L I_1 + \boldsymbol{\Omega} \cdot \frac{\partial I_0}{\partial \mathbf{x}} = 0 \quad (13.2)$$

$$L I_2 + \boldsymbol{\Omega} \cdot \frac{\partial I_1}{\partial \mathbf{x}} + \frac{\partial I_0}{\partial t} + q I_0 - q b \Phi = 0 \quad (13.3)$$

$$\frac{\partial \varphi}{\partial s} + L \varphi = 0 \quad (13.4)$$

$$\varphi(0; \mathbf{x}, \boldsymbol{\Omega}, \nu) + I_0(0, \mathbf{x}, \boldsymbol{\Omega}, \nu) = I^n. \quad (13.5)$$

Equation (13.1) yields

$$I_0 = b u_0, \quad \text{where } u_0 \text{ depends only on } \hat{t} \text{ and } \mathbf{x}.$$

Then (13.2) yields

$$I_1 = \frac{-b}{\sigma + \omega} \boldsymbol{\Omega} \cdot \frac{\partial u_0}{\partial \mathbf{x}} + b u_1, \quad \text{where } u_1 \text{ depends only on } \hat{t} \text{ and } \mathbf{x}.$$

And for the existence of the I_2 solution of (13.3) it is necessary and sufficient that

$$\left\langle \left\langle \boldsymbol{\Omega} \cdot \frac{\partial I_1}{\partial \mathbf{x}} \right\rangle \right\rangle + \frac{\partial u_0}{\partial \hat{t}} + \langle \langle q b \rangle \rangle (u_0 - \phi) = 0.$$

If one introduces the value of I_1 in this relationship, one obtains (12)(i). On the other hand, (13.4) and (13.5) give

$$\varphi = e^{-Ls}(I^{in} - bu_0(0)),$$

where e^{-Ls} denotes the semi-group whose generator is $-L$. Since $\varphi(s; \cdot) \rightarrow b\langle\langle I^{in} - bu_0(0) \rangle\rangle$ when s goes to ∞ , one sees that φ will be an initial layer term if and only if

$$u_0(0) = \langle\langle I^{in} \rangle\rangle.$$

So one obtains (12)(iii). Moreover, (12)(ii) is the condition which is compatible with (10)(ii). Thus it is necessary that u_0 satisfy Eq. (12). With this choice of u_0 , it may be proved that

$$I_\varepsilon(\hat{t}, \cdot) - \left[bu_0(\hat{t}, \cdot) + \varphi\left(\frac{\hat{t}}{\varepsilon^2}; \cdot\right) \right] = O(\varepsilon).$$

To obtain the desired result, one has to take into account the terms which are of order ε , that is, it is necessary to have

$$LI_3 + \mathbf{\Omega} \cdot \frac{\partial I_2}{\partial \mathbf{x}} + \frac{\partial I_1}{\partial t} + qI_1 = 0. \tag{13.6}$$

Moreover, for any \bar{x} on the boundary ∂D , the function $\psi(\xi; \hat{t}, \bar{x}, \mathbf{\Omega}, v)$ has to satisfy

$$\begin{aligned} \mathbf{\Omega} \cdot \mathbf{n}_x \frac{\partial \psi}{\partial \xi} + L\psi &= 0 \\ \psi(0; \hat{t}, \bar{x}, \mathbf{\Omega}, v) + I_1(\hat{t}, \bar{x}, \mathbf{\Omega}, v) &= 0 \quad \text{if } \mathbf{\Omega} \cdot \mathbf{n}_x \leq 0. \end{aligned} \tag{14}$$

The solvability condition for (13.6) gives (12')(i) and the condition for $\lim_{\xi \rightarrow \infty} \psi(\xi; \cdot) = 0$ gives (12')(ii). Thus it is necessary that u_1 satisfy Eq. (12'). With these choices of u_0 and u_1 , it may be proved that I_{rem} is a $O(\varepsilon^2)$ term.

One can now check that $u_0 + \varepsilon u_1 = u + O(\varepsilon^2)$, where u is the solution of the diffusion equation

$$\begin{aligned} \text{(i)} \quad \frac{\partial u}{\partial \hat{t}} - \frac{1}{3\sigma_0} \Delta u + q_P(u - \Phi) &= 0 \\ \text{(ii)} \quad u + \varepsilon \frac{L_0}{\sigma_0} \frac{\partial u}{\partial n} &= 0 \quad \text{on } \partial D \\ \text{(iii)} \quad u(0, \mathbf{x}) &= \langle\langle I^{in} \rangle\rangle. \end{aligned} \tag{15}$$

The boundary condition (15)(ii) (called Robin's boundary condition) means that the diffusion approximation is more accurate if we introduce an extrapolation

length (here, $\varepsilon(L_0/\sigma_0)$). This fact has been well known for a long time when one approximates a classical transport equation by a diffusion equation (this has been rigorously proved in Bardos–Santos–Sentis [5]).

The diffusion coefficient is not exactly equal to Rosseland's coefficient. In fact the approximation principles are different in both cases: Here the temperature is assumed to be constant on D ; in Rosseland's approximation there is equilibrium (up to order $O(\varepsilon)$) between material and radiation (see, e.g., Badham–Larsen–Pomraning [6]).

Since the angular dependency is not crucial, we may drop the term $(\Omega(\partial u_0/\partial x))$ whose integral over S^2 is zero. Since the boundary layer term may be dropped also, we obtain

$$I_\varepsilon(\hat{t}, \mathbf{x}, \boldsymbol{\Omega}, \nu) \simeq u(t, \mathbf{x}) b(\nu) + e^{-L\hat{t}/\varepsilon^2} (I^{\text{in}} - b \langle\langle I^{\text{in}} \rangle\rangle) \quad \text{with } u \text{ a solution of (15).} \quad (16)$$

2.2. Improvement of the Approximation

For the sake of simplicity we now drop the right-hand-side term of (10)(i). (As a matter of fact in the sequel (cf. Sect. 3) we only use the previous result in this case).

Since an accurate estimation of the absorbed energy (i.e., $\int_0^{\hat{t}} \int_D \langle\langle q I_\varepsilon(t, \mathbf{x}) \rangle\rangle dx dt$) is required, the previous approximation (16) may be quite crude. Indeed if there is no spatial variation of I_ε , i.e., if $I_\varepsilon = I_\varepsilon(\hat{t}, \nu)$ satisfies

$$\begin{aligned} \frac{\partial I_\varepsilon}{\partial \hat{t}} + \frac{1}{\varepsilon^2} L I_\varepsilon + q I_\varepsilon &= 0 \\ I_\varepsilon(0, \nu) &= I^{\text{in}}, \end{aligned} \quad (17)$$

then the previous approximation yields

$$I_\varepsilon(\hat{t}, \nu) = b(\nu) u(\hat{t}) + e^{-L\hat{t}/\varepsilon^2} [I^{\text{in}} - b \langle\langle I^{\text{in}} \rangle\rangle] + O(\varepsilon^2),$$

where

$$\begin{aligned} \frac{du}{d\hat{t}} &= q_{\text{P}} u \\ u(0) &= \langle\langle I^{\text{in}} \rangle\rangle. \end{aligned}$$

But it is easy to find the ε^2 corrector for I_ε ,

$$I_\varepsilon(\hat{t}, \nu) = \tilde{u}(\hat{t}) b(\nu) + \varepsilon^2 \tilde{\chi}(\hat{t}) \chi(\nu) + e^{-L\hat{t}/\varepsilon^2} [I^{\text{in}} - b \langle\langle I^{\text{in}} \rangle\rangle] + O(\varepsilon^4)$$

(up to an ε^2 initial layer term), where

$$\chi(\nu) = q_{\text{P}} b(\nu) \left(\frac{1}{\sigma} - \frac{1}{\sigma_{\text{M}}} \right) \quad \text{with} \quad \frac{1}{\sigma_{\text{M}}} = \left\langle\left\langle \frac{b}{\sigma} \right\rangle\right\rangle$$

and \tilde{u} satisfies

$$\begin{aligned} \frac{\partial \tilde{u}}{\partial \hat{t}} + \tilde{u} \left[q_P + \varepsilon^2 \left(\frac{q_P}{\sigma_P} - \frac{q_P}{\sigma_M} \right) \right] &= 0 \\ \tilde{u}(0) &= \langle\langle I^{in} \rangle\rangle + \varepsilon^2 \left[q_P \left\langle\left\langle \frac{I^{in}}{\sigma} \right\rangle\right\rangle - \frac{q_P}{\sigma_M} \langle\langle I^{in} \rangle\rangle \right]. \end{aligned} \tag{18}$$

Using this remark, we can improve the result of Proposition 1, and instead of (16) we take

$$I_\varepsilon(\hat{t}, \mathbf{x}, \mathbf{\Omega}, v) \simeq \hat{u}(\hat{t}, \mathbf{x}) b(v) + \varepsilon^2 \hat{u}(\hat{t}, \mathbf{x}) \chi(v) + e^{-L\hat{t}/\varepsilon^2} [I^{in} - b \langle\langle I^{in} \rangle\rangle], \tag{19}$$

where \bar{u} is the solution of the equation

$$\begin{aligned} \frac{\partial \hat{u}}{\partial \hat{t}} - \frac{1}{3\sigma_0} \Delta_x \hat{u} + \left[q_P + \varepsilon^2 \left(\frac{q_P}{\sigma_P} - \frac{q_P}{\sigma_M} \right) \right] \hat{u} &= 0 \quad \text{in } D \\ \hat{u} + \varepsilon \frac{L_0}{\sigma_0} \frac{\partial \hat{u}}{\partial n} &= 0 \quad \text{on } \partial D \\ \hat{u}(0, \mathbf{x}) &= \langle\langle I^{in} \rangle\rangle + \varepsilon^2 \left[q_P \left\langle\left\langle \frac{I^{in}}{\sigma} \right\rangle\right\rangle - \frac{q_P}{\sigma_M} \langle\langle I^{in} \rangle\rangle \right]. \end{aligned} \tag{20}$$

Now we write the result (19) with the help of the original variable t . Thus the coefficients σ_0 and σ_M are changed into

$$\begin{aligned} \sigma_{RW} &= \left\langle\left\langle \frac{b}{(1-l)k_a + k_{Th}} \right\rangle\right\rangle^{-1} \\ k_M &= \left\langle\left\langle \frac{b}{k_a} \right\rangle\right\rangle^{-1}. \end{aligned} \tag{21}$$

We can check that the Robin boundary condition is equivalent (up to a $O(\varepsilon^2)$ term) to a Dirichlet condition on an extended domain $\bar{D} = \{\mathbf{x} \in R^3 / \text{dist}(\mathbf{x}, D) \leq L_0 \sigma_{RW}^{-1}\}$. And we have

$$I(t, \mathbf{x}, \mathbf{\Omega}, v) = \bar{u}(t, \mathbf{x}) \bar{b}(v) + e^{-Lct/\varepsilon} (I^{in} - b \langle\langle I^{in} \rangle\rangle), \tag{22}$$

where \bar{u} is the solution of

$$\begin{aligned} \frac{1}{c} \frac{\partial \bar{u}}{\partial t} - \frac{1}{3\sigma_{RW}} \Delta_x \bar{u} + l \langle\langle k_a \bar{b} \rangle\rangle \bar{u} &= 0 \quad \text{in } \bar{D} \\ \bar{u} &= 0 \quad \text{on } \partial \bar{D} \\ \bar{u}(0, \mathbf{x}) &= \langle\langle I^{in} \rangle\rangle I_* \end{aligned} \tag{23}$$

with

$$\begin{aligned}\bar{b}(v) &= b(v) + \frac{l}{1-l} k_P \left(\frac{b(v)}{k_a(v)} - \frac{b(v)}{k_M} \right) \\ I_* &= 1 - \frac{l}{1-l} \left(\frac{k_P}{k_M} - \frac{k_P}{\langle\langle I^{in} \rangle\rangle} \left\langle\left\langle \frac{I^{in}}{k_a} \right\rangle\right\rangle \right).\end{aligned}\tag{24}$$

We can now estimate the energy absorbed during the time interval $[0, t^1]$ with the formulation (22),

$$\begin{aligned}\int_0^{t^1} \langle\langle \sigma_a I(t, \mathbf{x}) \rangle\rangle dt &= l \langle\langle k_a \bar{b} \rangle\rangle \int_0^{t^1} \bar{u}(t, \mathbf{x}) dt \\ &\quad + \frac{\varepsilon}{c} \left\langle\left\langle \int_0^{ct^1/\varepsilon} \sigma e^{-Ls} (I^{in} - b \langle\langle I^{in} \rangle\rangle) ds \right\rangle\right\rangle \\ &\simeq l \langle\langle k_a \bar{b} \rangle\rangle \int_0^{t^1} \bar{u}(t, \mathbf{x}) dt \\ &\quad + \frac{\varepsilon^2}{c} \left\langle\left\langle q \int_0^{+\infty} e^{-Ls} (I^{in} - b \langle\langle I^{in} \rangle\rangle) ds \right\rangle\right\rangle.\end{aligned}$$

But it is easy to show that

$$\varepsilon^2 \left\langle\left\langle q \int_0^{+\infty} e^{-Ls} (I^{in} - b \langle\langle I^{in} \rangle\rangle) ds \right\rangle\right\rangle = \frac{l}{1-l} k_P \left(- \left\langle\left\langle \frac{I^{in}}{k_a} \right\rangle\right\rangle + \left\langle\left\langle \frac{I^{in}}{k_M} \right\rangle\right\rangle \right).$$

We can conclude that

$$\int_0^{t^1} \langle\langle \sigma_a I(t, \mathbf{x}) \rangle\rangle dt \simeq l \langle\langle k_a \bar{b} \rangle\rangle \int_0^{t^1} \bar{u}(t, \mathbf{x}) dt + \frac{1}{c} [\langle\langle I^{in} \rangle\rangle - \bar{u}(0, \mathbf{x})].\tag{25}$$

So we shall obtain the same estimation for the absorbed energy if, instead of (22), we use $I(t, \mathbf{x}, \boldsymbol{\Omega}, \nu) \simeq \bar{I}(t, \mathbf{x}, \boldsymbol{\Omega}, \nu)$, where

$$\bar{I}(t, \mathbf{x}, \boldsymbol{\Omega}, \nu) = \bar{u}(t, \mathbf{x}) \bar{b}(\nu) \quad \text{for } t > 0, \text{ with } \bar{u} \text{ solution of (23),}\tag{26}$$

and if we take (25) into account.

3. DIFFUSION APPROXIMATION OF THE TRANSPORT EQUATION SATISFIED BY A MONTE CARLO PARTICLE

Let us recall the main outlines of the classical Monte Carlo method to solve (4). On the time step $[0, t^1]$ particles are emitted from the source S (including volume emission, boundary emission, and initial radiation energy) and are tracked from

collision to collision until the time t^l . Formally this corresponds to a random walk $\mathbf{R}_0 \rightarrow \mathbf{R}_1 \rightarrow \dots \rightarrow \mathbf{R}_k$ in the phase space $\mathcal{R} = \{\mathbf{R} = (t, \mathbf{x}, \boldsymbol{\Omega}, \nu)\}$, each point corresponds to collision, census, or escape event.

3.1. The Transport Equation for a Particle

We take an interest here in only one Monte Carlo photon already emitted. For the sake of simplicity we suppose the particle to be emitted at time $t_0 = 0$, at point \mathbf{x}_0 with an energy (or weight) $e_0 = 1$. The initial direction $\boldsymbol{\Omega}_0$ is supposed to be uniformly distributed on the unit sphere S^2 and the frequency ν_0 is sampled from a given probability $f(\nu)$ on $]0, +\infty[$.

Since the diffusion approximation needs a constant temperature in the whole domain, we must track the particle in a part D included in the cell containing \mathbf{x}_0 . The transport problem corresponding to this photon is then Eq. (4), without the right-hand-side term of (4)(i), that is,

$$\frac{1}{c} \frac{\partial I}{\partial t} + \boldsymbol{\Omega} \cdot \frac{\partial I}{\partial \mathbf{x}} + k_a I + k_{\text{Th}} QI - \frac{k_a b}{k_p} \int_0^\infty \int_{S^2} \sigma_s(\nu') I(\boldsymbol{\Omega}', \nu') \frac{d\boldsymbol{\Omega}'}{4\pi} d\nu' = 0$$

$$I = 0 \quad \text{if } (\mathbf{x}, \boldsymbol{\Omega}) \in \partial D^- \tag{27}$$

$$I(0, \mathbf{x}, \boldsymbol{\Omega}, \nu) = c\delta(\mathbf{x} - \mathbf{x}_0) \frac{1}{4\pi} f(\nu) \quad (\delta \text{ is the Dirac distribution}).$$

The emission and tracking of the photons are equivalent to the sampling of a random walk $\{\mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_j, \dots\}$ related to a probability p computed from the source $S(\mathbf{R}_0)$ and the stochastic kernel $(\mathbf{R}_j \rightarrow \mathbf{R}_{j+1})$ (see Spanier-Gelbard [7]). The relation between this probability p on the space of random walks and the intensity I solution of (27) is given by the following:

For every function G on \mathcal{R} , we can construct a random variable g , such that

$$E_p[g] = \int_{\mathcal{R}} G(\mathbf{R}) I(\mathbf{R}) d\mathbf{R},$$

where $E_p[g]$ is the expected value of g with respect to p .

For our purpose there are three very important random variables. These are defined at a time corresponding to an event of the tracking, i.e., at a time t_j of the random walk $\{\mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_j, \dots\}$ (it is always possible to stop the photon at t_j for computing these estimators and to continue the tracking since this is a Markov process).

Radiation energy (or weight) at time t_j ,

$$e(t_0) = 1$$

$$e(t_j) = e(t_{j-1}) \exp\{-\sigma_a(\nu_{j-1}) c(t_j - t_{j-1})\}$$

$$e(t_j) = 0 \quad \text{if } \mathbf{x}_j \notin D.$$

Absorbed energy on $[0, t_j]$,

$$e_{\text{abs}}(t_j) = 1 - e(t_j) \\ = \prod_{i=1}^j [1 - \exp\{-\sigma_a(v_{i-1}) c(t_i - t_{i-1})\}] \quad \text{if } \mathbf{x}_j \in D.$$

Number of particles at time t_j ,

$$e_0(t_j) = 1 \quad \text{if } \mathbf{x}_j \in D \\ e_0(t_j) = 0 \quad \text{if } \mathbf{x}_j \notin D.$$

These three random variables have the following expected values:

Radiation energy on D at time t ,

$$E_p[e(t)] = E_R(t) = \frac{1}{c} \int_D d\mathbf{x} \int_0^\infty dv \int_{S^2} d\Omega I(\mathbf{R}).$$

Absorbed energy in $D \times [0, t]$,

$$E_p[e_{\text{abs}}(t)] = E_{\text{abs}}(t) = \int_0^t ds \int_D d\mathbf{x} \int_0^\infty dv \int_{S^2} d\Omega \sigma_a(v) I(s, \mathbf{x}, \Omega, v).$$

Average number of particles in D at time t ,

$$E_p[e_0(t)] = E^0(t) = \frac{1}{c} \int_D d\mathbf{x} \int_0^\infty dv \int_{S^2} d\Omega I^0(\mathbf{R}),$$

where I^0 is the solution of the transport problem (27) without the absorption term

$$\frac{1}{c} \frac{\partial I^0}{\partial t} + \Omega \cdot \frac{\partial I^0}{\partial \mathbf{x}} + k_{\text{Th}} Q I^0 + \sigma_s I^0 - \frac{k_a b}{k_p} \int_0^\infty \int_{S^2} \sigma_s(v') I^0(\Omega', v') \frac{d\Omega'}{4\pi} dv' = 0.$$

3.2. The Diffusion Approximation

Let us now write the diffusion approximation of Eqs. (27) given by (26). We introduce the function $\tilde{u}(t, \mathbf{x})$ solution of the diffusion equation

$$\frac{1}{c} \frac{\partial \tilde{u}}{\partial t} - \frac{1}{3\sigma_{\text{RW}}} \Delta_x \tilde{u} = 0, \quad \mathbf{x} \in \bar{D} \\ \tilde{u} = 0, \quad \mathbf{x} \in \partial \bar{D} \\ \tilde{u}(0, \mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0). \quad (28)$$

Let us define

$$\tilde{\sigma}_P = \int_0^\infty l k_a(v) \tilde{b}(v) dv = l k_P \left[1 + \frac{l}{1-l} \left(1 - \frac{k_P}{k_M} \right) \right].$$

The specific energy I supposed to be isotrope, is then approximated for $t > 0$, by

$$\tilde{I}(t, \mathbf{x}, \Omega, \nu) = \frac{c}{4\pi} I_* e^{-\tilde{\sigma}_P c t} \tilde{b}(\nu) \tilde{u}(t, \mathbf{x}). \tag{29}$$

Interpretation

We can see from Eq. (29) that, when the approximation is feasible, the weight of the photon is

$$e(t) = I_* \exp\{-\tilde{\sigma}_P c t\}$$

and the frequency is distributed according to $\tilde{b}(\nu)$ which is, to first order, the normalized Planck function $b(\nu)$. The position \mathbf{x} at time t is distributed according to $\tilde{u}(t, \mathbf{x})$.

Because we have removed the initial layer, we must make this approximation only when time t is large enough. Consequently there is a discontinuity for $t = 0$ in the expression of \tilde{I} : the weight of the photon ($e_0 = 1$ at $t = 0$) becomes I_* when $t \rightarrow 0^+$, $t \neq 0$. We can say that this jump comes from the modification of the frequency spectrum ($f(\nu)$ at $t = 0$ becomes $\tilde{b}(\nu)$ at $t \neq 0$). The difference $(1 - I_*)$ is added to the absorption energy into D as shown in Section 2 (Figs. 1 and 2).

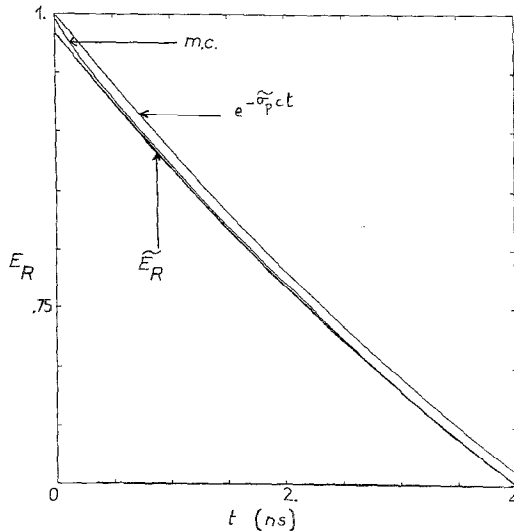


FIG. 1. The domain D is assumed to be R^3 . Here $k_a(\nu) = C\nu^3 \exp(-\nu/T)$; $f(\nu) = k_a(\nu) \cdot b(\nu) k_P^{-1}$; $l = 10^{-3}$. The Monte Carlo solution of problem (27) is compared with the diffusion approximation $\tilde{E}_R(t) = I_* \exp(-\tilde{\sigma}_P c t)$ and with $\exp(-\tilde{\sigma}_P c t)$.

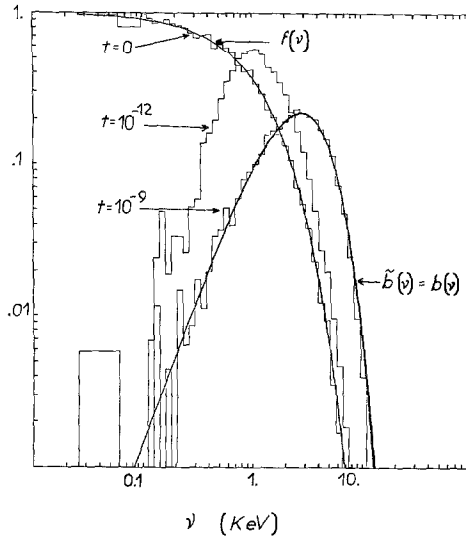


FIG. 2. With the same assumptions as in Fig. 1, we plot the frequency spectrum at time $t=0$, $t=10^{-12}$ s and $t=10^{-9}$ s.

3.3. Explicit Solution of the Diffusion Equation

We now assume D to be a sphere of \mathbb{R}^3 with center \mathbf{x}_0 . Since the temperature must be constant in the domain D , D will be the largest sphere with center \mathbf{x}_0 included into the cell. We denote by R_0 the radius of D , $\bar{R}_0 = R_0 + L_0 \sigma_{RW}^{-1}$ the radius of \bar{D} and $r = \|\mathbf{x} - \mathbf{x}_0\|$ the spherical variable.

The solution \tilde{u} of the diffusion equation (28) in \bar{D} is

$$\tilde{u}(t, r) = \frac{1}{2\bar{R}_0^2} \sum_{n=1}^{\infty} \frac{n}{r} \sin\left(\frac{n\pi r}{\bar{R}_0}\right) A^{n^2},$$

where

$$A = \exp\left\{-\frac{ct}{3\sigma_{RW}} \frac{\pi^2}{\bar{R}_0^2}\right\}.$$

We introduce the two functions

$$\begin{aligned} F(t, R) &= \int_0^R \tilde{u}(t, r) 4\pi r^2 dr \\ &= \frac{2}{\pi} \sum_{n=1}^{\infty} A^{n^2} \left(-X \cos nX + \frac{\sin nX}{X}\right), \end{aligned}$$

where $X = \pi R/\bar{R}_0$, and

$$P(t) = F(t, \bar{R}_0) = 2 \sum_{n=1}^{\infty} (-1)^{n+1} A^{n^2}.$$

$P(t)$ is the average number of particles in \bar{D} at time t and the function $R \rightarrow F(t, R)/P(t)$ is the spatial distribution of particles in the sphere at time t .

Thereafter we shall use $P(t)$ instead of $F(t, R_0)$. The difference between these two quantities is small and $P(t)$ has the advantage of depending only on one parameter. We can then write the radiation energy and the absorbed energy using only $P(t)$,

$$\tilde{E}_r(t) = I_* e^{-\bar{\sigma}_p c t} P(t)$$

$$\tilde{E}_{\text{abs}}(t) = (1 - I_*) + I_* \int_0^t c \bar{\sigma}_p e^{-\bar{\sigma}_p c s} P(s) ds.$$

Let us recall that the first term $(1 - I_*)$ comes from the jump at $t=0$ of the radiation energy, i.e., of the integration of the initial layer.

4. THE RANDOM WALK PROCEDURE

4.1. Criteria for Random Walk

We must determine empirically the domains of validity of the diffusion approximation of Fleck's transport equation in a sphere. To do this, we compare the solution of (27) calculated using Fleck's Monte Carlo method with the exact solution given in Section 3.3. A priori, these conditions are:

—The coefficient l must be small enough to satisfy the assumption (7) and to allow the asymptotic expansions in ϵ .

—We must observe the tracking at a time large enough (see Sect. 3.2).

—The radius R_0 of the sphere D must be large (compared to σ_{RW}^{-1}) in order to satisfy the assumption (6).

The extrapolation coefficient L_0 is determined by comparing the numerical solution of (27) with the family u_{L_0} depending on the parameter L_0 . When the macroscopic absorption cross-section k_a does not depend on the frequency and when there is no Thomson scattering ($k_{\text{Th}} = 0$), the coefficient L_0 was calculated by Chandrasekhar [8] and the numerical tests give us the same value $L_0 = 0.71$.

We will study with particular care the case of analytical opacities without Thomson scattering,

$$k_a(\nu) = \frac{\text{constant}}{\nu^3} \left(1 - \exp \left\{ - \frac{h\nu}{KT} \right\} \right),$$

$$k_{\text{Th}} = 0.$$

We will consider three different distributions of the initial frequency

$$\begin{aligned}
 f(v) &= b(v) && \text{[then } I_* = 1 \text{]} \\
 f(v) &= \frac{k_a(v) b(v)}{k_p}; && \left[I_* = 1 + \frac{l}{1-l} \left(1 - \frac{k_p}{k_M} \right) \simeq 1 - 16.39 \frac{l}{1-l} \right] \\
 f(v) &= \delta(v - v_0); && \left[I_* = 1 + \frac{l}{1-l} \left(\frac{k_p}{k_a(v_0)} - \frac{k_p}{k_M} \right) \right].
 \end{aligned}$$

We can see that the frequency is distributed according to $\tilde{b}(v) \simeq b(v)$ when the diffusion approximation is suitable. The first distribution $f(v)$ corresponds to a particle we track just after its random walk. The second distribution is exactly the frequency spectrum of a particle emitted in the cell during the time step. It is also the distribution of a photon just after a Fleck collision. When the frequency of a particle is not distributed according to these two functions (e.g., when the particle comes from another cell) we used the Dirac $\delta(v - v_0)$, where v_0 is the frequency of the photon.

The numerical tests show that the extrapolation coefficient is around 2, and that the diffusion approximation is suitable when using the criteria (Figs. 3-5),

$$l \leq 0.01$$

$$R_0 \geq 5\sigma_{RW}^{-1}$$

and

$$R_0 \geq 5\sigma_S^{-1}(v_0) \quad \text{if } f(v) = \delta(v - v_0).$$

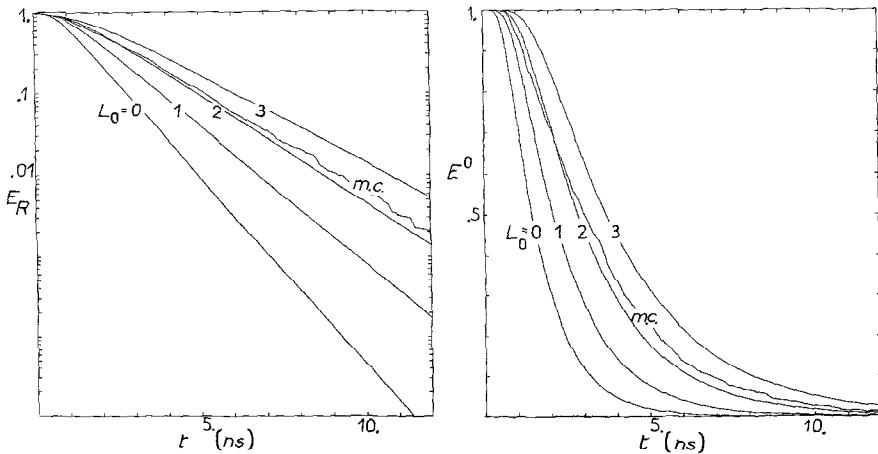


FIG. 3. Estimation of the extrapolation length. Comparison between Monte Carlo estimation and diffusion approximation (for various values of L_0) of the number of particles $E^0(t)$ and the radiative energy $E_R(t)$. Here D is a sphere of radius $5\sigma_{RW}^{-1}$ and $l = 10^{-3}$.

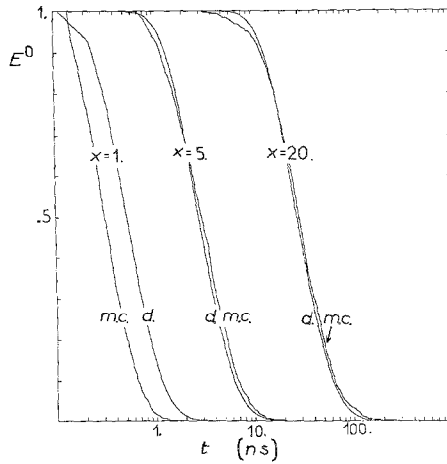


FIG. 4. Domain of validity. Comparison between Monte Carlo estimation and diffusion approximation of the number of particles $E^0(t)$. D is a sphere of radius $x\sigma_{RW}^{-1}$ with $l = 10^{-3}$ and $L_0 = 2$.

The last criterion ensures that the photon with initial frequency ν_0 has a first Fleck collision near the center of the sphere. (The particles of high frequency, emitted, for example, from a hot black body, go through the cell without Fleck collisions and they do not satisfy this criterion.)

The tests prove that the frequency spectrum tends to $b(\nu)$ very quickly and that the term I_* in the expression of the energy yields a more accurate result, without any additional computation.

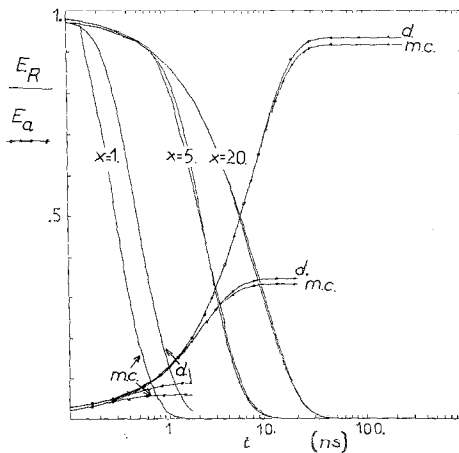


FIG. 5. Comparison between Monte Carlo and diffusion approximation of the radiative energy $E_R(t)$ and the absorption energy $E_a(t)$ with the same value as in Fig. 4.

4.2. Description of the Random Walk Procedure

The random walk procedure is grafted on the Monte Carlo method without distinction between optically thin or optically thick medium. At the beginning of the tracking of each photon (going from an event R_{j-1} to another R_j) we calculate the greatest sphere D with center x_{j-1} included in the cell and we test the random walk criteria. If they are satisfied we sample the escape time τ from D according to the distribution $1 - P(\tau)$. The absolute escape time is then $\theta = t_{j-1} + \tau$.

If θ is less than the end of the time step, the particle's position x_j is sampled uniformly on the boundary ∂D , the frequency ν_j according to $b(\nu)$, the direction Ω_j is distributed according to Lambert's law outside of the sphere and the new weight is

$$e_j = e_{j-1} I_* \exp\{-\bar{\sigma}_p c(t_j - t_{j-1})\}.$$

If θ is not in the time interval, we stop the photon at the end of this one. The radius r is sampled with the repartition $F(t, r)/P(t)$ in $[0, R_0]$ and the position x_j is uniformly distributed on the sphere of radius r . Then ν_j is sampled according to $b(\nu)$, Ω_j is uniformly distributed on S^2 and the weight e_j is calculated as previously. (Note that the procedure is the same as in [2] and [3]; however, our diffusion approximation is not the same except for coefficient σ_{RW} ; moreover the sample of frequency and escape time, and the calculus of the absorption energy are not identical.)

5. NUMERICAL RESULTS

We now present a numerical example with the random walk procedure. It is a problem described in Fleck-Cummings [1]: A slab of thickness 4 cm, with an optically thick medium between 2 and 2.4 cm is heated by a black body source. The spatial step size is $\Delta x = 0.4$ cm and the cross sections are

$$k_{Th} = 0$$

$$k_a = \frac{27}{\nu^3} \left(1 - \exp\left\{-\frac{\nu}{T}\right\} \right) \quad \text{if } \nu \text{ and } T \text{ are given in kilo-electron-volts.}$$

In the sixth cell, the macroscopic cross-section k_a is multiplied by a factor of 1000. (Note that it is not the factor used in Fleck-Cummings [1].) The boundary conditions are

- Black body emission with $T = 1$ Kev in $x = 0$ cm.
- Purely absorbing medium for $x \geq 4$ cm.
- Initial temperature $T_0 = 0.001$ Kev.

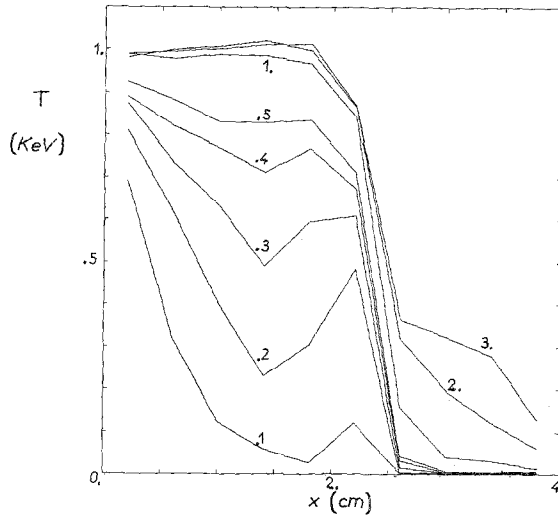
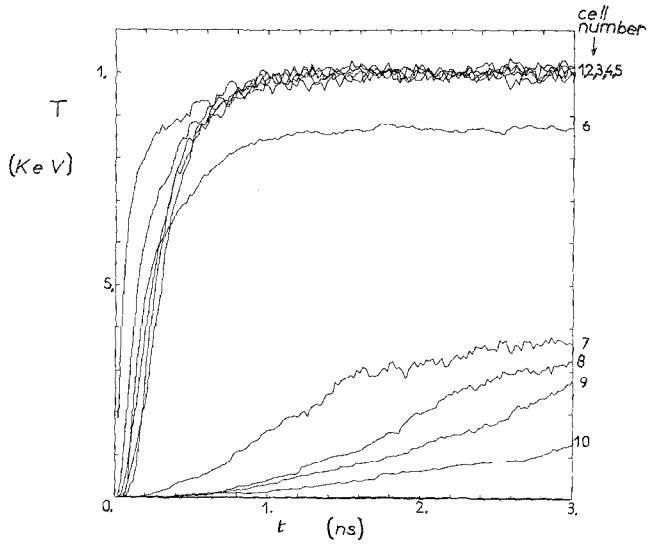


FIG. 6. Temperature T versus time in the ten cells using computation (b) and temperature versus space at different times.

The medium is supposed to be a perfect gas. The specific energy \mathcal{E} is given by the equation of state

$$\mathcal{E} = 6.9913 \cdot 10^6 \times T \quad (\text{in CGS units}).$$

We have compared three computations:

- (a) Fleck's Monte Carlo method, without random walk.
- (b) Random walk with $L_0 = 2$ and the criterion $R_0 \geq 5\sigma_{RW}^{-1}$,
- (c) Random walk with $L_0 = 0$ and the criterion $R_0 \geq 20\sigma_{RW}^{-1}$.

The results are the same up to the statistical fluctuations.

At time $t = 1$ ns ($1 \text{ ns} = 10^{-9}$ sec), with time step $\Delta t = 0.02$ ns, we have

	(a)	(b)	(c)
Computer time	3 h 04 min	6 min	22 min
Number of particles	13,233	13,381	13,355
Number of Fleck's scattering	379×10^6	11×10^6	44×10^6
Number of random walk procedures	0	89,000	59,000

Remark 1. The random walk procedure with $L_0 = 0$ and the criterion $R_0 \geq 5\sigma_{RW}^{-1}$ gave us wrong results: the extrapolation length is essential.

Remark 2. Fleck's coefficient l is very small in the opaque medium ($l \simeq 5 \times 10^{-4}$). Hence it follows that $\tilde{\sigma}_p \simeq lk_p$.

Conclusion

The diffusion approximation of Fleck's transfer equation given by the multiple scales technique is well satisfied by the numerical tests, hence the random walk procedure which has been described is reliable when the criteria of validity are satisfied.

The method which has been described here for Fleck's equation may be used for other equations where the streaming terms are the most important except in a collisional region in which the scattering term is very important, e.g., in the Fokker-Planck equation for charged particles in a plasma. The crucial point of the method is to find an accurate limit of the solution of the considered equation in a collisional region such that this limit function may be computed very easily for a simple geometry.

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