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PRINCIPLE OF THE RANDOM WALK METHOD FOR RADIATIVE TRANSFER EQUATIONS AND APPLICATION

Part 2 : Application to Fleck's Monte-Carlo method

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J. GIORLA

INTRODUCTION

The Fleck's Monte-Carlo method is used to solve time-dependent non linear transport problems in optically thin or optically thick media (Fleck-Cumming [1]). One part of the absorption-emission process is replaced by a scattering process via the introduction of the so-called Fleck collision term. The variance of the temperature does not increase when the time step becomes large and the method is unconditionally stable in the grey case (Mercier [1]). However, when there is a region of high opacity the number of scattering events increases which becomes time consuming. In this paper we shall use the Random Walk procedure to accelerate the tracking of the particles which have a large number of collision events. This method is based on the approximation of Fleck's transport equation by a diffusion equation using the multiple scale technique described in part I.

The chapter is organized as follows.

In Sec. 1 we derive the transfer equation satisfied by a Monte-Carlo particle and the corresponding diffusion equation, the explicit solution of which is known in a sphere. We calculate the probability of escaping from the sphere and the probability of remaining inside at the end of the time step in Sec. 2. We study some criteria for the validity of this approximation in Sec. 3, using Monte-Carlo calculations in the sphere. Numerical results are given in Sec. 4.

II.1 - DIFFUSION APPROXIMATION OF THE TRANSPORT EQUATION SATISFIED BY A MONTE-CARLO PARTICLE

- As we want to accelerate the tracking of a particle, it is necessary to describe the tracking itself. On the time step $[t_0, t_1]$ particles are emitted from the radiation emission source S (S includes volume emission, boundary emission and initial radiation energy) and are tracked from collision to collision until the end of the time step. Formally particles proceed from source to termination through a series of points $R_0 \to R_1 \to \ldots R_k$ in phase space $\mathcal{P} = \{R = (t,x,\Omega,\nu)\}$, each point R_i corresponding to collision census or escape events (the absorption is treated by exponential attenuation).

We denote by $K(R' \to R)$ the transfer kernel from R' to R so that the specific energy I satisfies the integral transport equation

$$I(R) = \int_{\mathcal{P}} K(R' \to R)\, I(R')\, dR' + S(R).$$

This formal equation is the integral form of the Fleck's transport equation used in part I.

- We are interested 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 x_0 with an energy (or weight) $e_0 = 1$. The initial direction Ω_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 $]0,+\infty[$.

- As 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 x_0. The transport problem corresponding to this photon is then :

. Fleck's transport equation without emission in D,
. initial intensity given by the distribution of R_0,
. absorption condition on the boundary.

We can now write the equation corresponding to this particle with the notations defined in part I :

(II.1)
$$\begin{cases} \frac{1}{c}\frac{\partial I}{\partial t} + \Omega \frac{\partial I}{\partial x} + k_a I + k_s QI = \iint \sigma_s(\nu' \to \nu)\, I(\Omega',\nu')\, \frac{d\Omega'}{4\pi}\, d\nu' \\ I(0,x,\Omega,\nu) = c\ \delta(x - x_o)\ \frac{1}{4\pi} f(\nu) \\ I = 0 \quad \text{if } (x,\Omega) \in \partial D_- \end{cases}$$

The emission and tracking of the photons are equivalent to the sampling of a random walk $c = \{R_o \to R_1 \to .. R_k\}$ from a probability p computed from the source $S(R_o)$ and the kernel $K(R_{j-1} \to R_j)$ (cf. Spanier-Gelbard [1]). The relation between this probability p on the space of random walks $\mathcal{C}$ and the intensity I solution of (II.1) is given by the following :

For every fonction F on $\mathcal{V}$, we can construct a random variable f on $\mathcal{C}$ such that :

$$E[f] = \int_{\mathcal{V}} F(R)\ I(R)\ dR$$

where $E[f]$ is the expected value of f 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 $\{R_o \to R_1 \ldots R_j \ldots R_k\}$ (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).

<u>Radiation energy (or weight) at time t_j</u>

$$e(t_o) = 1$$
$$e(t_j) = e(t_{j-1}) \exp\{-\sigma_a(\nu_{j-1})\ c\ (t_j - t_{j-1})\}$$
$$e(t_j) = 0 \text{ if } x_j \notin D$$

<u>Absorption energy on</u> $[0, t_j]$

$$e_{abs}(t_j) = 1 - e(t_j)$$
$$= \prod_{i=1}^{j} [1 - \exp\{-\sigma_a(\nu_{i-1})\ c(t_i - t_{i-1})\}]$$
$$\text{if } x_j \in D$$

Number of particles at time t_j

$e_o(t_j) = 1$ if $x_j \in D$
$e_o(t_j) = 0$ if $x_j \notin D$

These three random variables have the following expected values :

Radiation energy on D at time t

$$E[e(t)] = E_R(t) = \frac{1}{c} \int_D dx \int_0^\infty d\nu \int_{S^2} d\Omega \quad I(R)$$

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

$$E[e_{abs}(t)] = E_{abs}(t) = \int_0^t ds \int_D dx \int_0 d\nu \int_{S^2} d\Omega\ \sigma_a(\nu)\ I(s,x,\Omega,\nu)$$

Average number of particles in D at time t

$$E[e_o(t)] = E^o(t) = \frac{1}{c} \int_D dx \int_0^\infty d\nu \int_{S^2} d\Omega\ I^o(R)$$

where I^o is the solution of the transport problem (II.1) without the absorption term :

$$\frac{1}{c} \frac{\partial I^o}{\partial t} + \Omega \frac{\partial I^o}{\partial x} + k_S\, \Omega I^o = \iint \sigma_s I^o \frac{d\Omega'}{4\pi} d\nu' - (1-p) k_a I^o$$

Let us now write the diffusion approximation of equations (II.1) using the multiple scales technique of part I. We introduce the function $\tilde{u}(t,x)$ solution of the diffusion equation :

$$\text{(II.2)} \quad \begin{cases} \frac{1}{c} \frac{\partial \tilde{u}}{\partial t} - \frac{1}{3\sigma_{RW}} \Delta \tilde{u} = 0 & x \in \bar{D} \\ \tilde{u} = 0 & x \in \overline{\partial D} \\ \tilde{u}(0,x) = \delta(x - x_o) & \end{cases}$$

where $\sigma_{RW}^{-1} = \int_0^\infty \frac{b(\nu)\, d\nu}{(1-\ell)\, k_a(\nu) + k_s(\nu)}$

$\bar{D} = \{x$; distance between x and D is less than $L_o\, \sigma_{RW}^{-1}\}$

L_o is the extrapolation coefficient introduced in part I.

We notice that, with the notations of part I

$$k_M^{-1} = \int_0^\infty k_a^{-1}(\nu)\, b(\nu)\, d\nu \quad ,$$

$$I_* = 1 - \frac{\ell}{1-\ell}\left[\frac{k_P}{k_M} - k_P \int_0^\infty \frac{f(\nu)\, d\nu}{k_a(\nu)}\right] \quad ,$$

$$\tilde{b}(\nu) = b(\nu)\left[1 + \frac{\ell}{1-\ell}\left(\frac{k_P}{k_a(\nu)} - \frac{k_P}{k_M}\right)\right] \quad ,$$

$$\tilde{\sigma}_P = \int_0^\infty \ell\, k_a(\nu)\, \tilde{b}(\nu)\, d\nu = \sigma_P\, [1 + \frac{\ell}{1-\ell}\,(1 - \frac{k_P}{k_M})]$$

Thus we have $\bar{u}(t,x) = \tilde{u}(t,x)\, e^{-\tilde{\sigma}_P ct}$ and $<<I_{in}>> = \frac{c}{4\pi}\, \delta_{x_o}$

The specific energy I supposed to be isotrope, is then approximated by :

(II.3) $$\boxed{\tilde{I}\,(t,s,\Omega,\nu) = \frac{c}{4\pi}\, I_*\, e^{-\tilde{\sigma}_P ct}\, \tilde{b}\,(\nu)\, \tilde{u}(t,x)\ ,\ t \neq 0\ .}$$

(We have used the approximation given in (I.26)).

Interpretation

- We can see from this last equation that, when the approximation is feasible, the weight of the photon is

$$e(t) = I_* \exp\{-\tilde{\sigma}_p\, ct\}$$

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

- Because we have removed the initial layer, we must make this approximation only when time t is large enough. A consequence is a discontinuity for t = 0 in the expression of $\tilde{I}$: the weight of the photon ($e_o = 1$ at t = 0) becomes I_* when $t \searrow 0^+$, $t \neq 0$. 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 part I (figures 1, 2).

II.2 - EXPLICIT SOLUTION OF THE DIFFUSION EQUATION

We now assume D to be a sphere of $\mathbb{R}^3$ with center x_o. As the temperature must be constant in the domain (see part I) D will be the largest sphere with center x_o included into the cell. We denote by R_o the radius of D, $\bar{R}_o = R_o + L_o \sigma_{RW}^{-1}$ the radius of $\bar{D}$ and $r = \|x-x_o\|$ the spherical variable.

The solution $\tilde{u}$ of the diffusion equation (II.2) in $\bar{D}$ is :

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

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

We introduce the two functions :

$$F(t,R) = \int_0^R \tilde{u}(t,r)\, 4\pi r^2\, dr$$

$$= \frac{2}{\pi} \sum_{n=1}^{\infty} A^{n^2} \left(-X \cos X + \sin \frac{nX}{X}\right),$$

where $X = \frac{\pi r}{\bar{R}_o}$, and

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

P(t) is the average number of particles being into $\bar{D}$ at time t and the function $R \to \frac{F(t,R)}{P(t)}$ is the spatial distribution function of particles into the sphere at t.

Thereafter we shall use P(t) instead of $F(t,R_o)$. 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 radiative energy and the absorption energy using only P(t) :

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

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

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.

II.3 - CRITERIA FOR RANDOM WALK

We have determined empirically the domains of validity of the diffusion approximation of Fleck's transport equation in a sphere. To do this, we compared the solution of (II.1) calculated using Fleck's Monte-Carlo method with the exact solution given in Sec. 2. A priori, these conditions are :

- The coefficient ℓ must be small enough to satisfy the assumption that σ_S/σ_a is small and to allow the asymptotic expansions in ε ;

- We must observe the tracking at a time large enough and on a large area, in particular the radius R_o of the sphere D must be large compared to σ_{RW}^{-1}.

The extrapolation coefficient L_o has been determined by comparing the numerical solution of (II.1) with the family u_{L_o} depending on the parameter L_o. When the macroscopic absorption cross section k_a does not depend upon the frequency and when there is no Thomson scattering ($k_S = 0$), the coefficient L_o was calculated by Chandrasekkar [1] and the numerical tests gave us the same value $L_o = .71$.

We have studied with particular care the case of analytical opacities without Thomson scattering :

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

$$k_S = 0$$

We have considered three possible distributions of the initial frequency :

$$f(\nu) = b(\nu) \qquad \left[\text{ then } I_* = 1 \right] ,$$

$$f(\nu) = \frac{k_a(\nu)\ b(\nu)}{k_P} \quad \left[I_* = 1 + \frac{\ell}{1-\ell} \left(1 - \frac{k_P}{k_M}\right) \simeq 1 - 16.39 \frac{\ell}{1-\ell} \right]$$

$$f(\nu) = \delta(\nu-\nu_o) \left[I_* = 1 + \frac{\ell}{1-\ell} \left(\frac{k_P}{k_a(\nu_o)} - \frac{k_P}{k_M} \right) \right] .$$

We have seen that the frequency is distributed according to $\tilde{b}(\nu) \simeq b(\nu)$ when the diffusion approximation is suitable. Thus the first distribution f (ν) 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 (that is, for example, when the particle comes from another cell) we used the Dirac $\delta(\nu-\nu_o)$ where ν_o is the frequency of the photon.

The numerical tests have shown that the extrapolation coefficient is around 2 and that the diffusion approximation is suitable when using the criteria (figures 3, 4, 5) :

$$\ell \leq .01$$

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

and $$R_o \geq 5\ \sigma_S^{-1}(\nu_o) \text{ if } f(\nu) = \delta(\nu-\nu_o) .$$

The last criterion ensures that the photon with initial frequency ν_o 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 criterium.

The tests have proven that the frequency spectrum tends to b (ν) very quickly and that the term I_* in the expression of the energy is essential.

II.4 - ACCELERATION OF FLECK'S MONTE-CARLO METHOD BY RANDOM WALK AND NUMERICAL RESULTS

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 a event R_{j-1} to another R_j) we calculate the greatest sphere with center x_{j-1} included in the cell and we test the Random Walk criteria. If these 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

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

- If θ is not in the time interval, we stop the photon at the end of it. The radius r is sampled with the repartition $\frac{F(t,r)}{P(t)}$ in $[0, R_o]$ 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 (Notice that the procedure is the same as in Fleck-Canfield [1] ; 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.)

– We now present a numerical example with the Random Walk procedure. It is a problem described in Fleck-Cumings [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 $\Delta x = .4$ cm and the cross-sections are :

$$k_S = 0 ,$$

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

In the sixth cell, the macroscopic cross-section k_a is multiplied by a factor 1000 (Note that it is not the opacity 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_o = .001 Kev.

The medium is supposed to be a perfect gas. The specific energy ε_m is given by the equation of state :

$$\varepsilon_m = 6.9913 \; 10^6 \; T \text{ in CGS units.}$$

We have compared three computations :

- Fleck's Monte-Carlo method,
- Random Walk with $L_o = 2$ and the criterium $R_o \geq 5\sigma_{RW}^{-1}$,
- Random Walk with $L_o = 0$ and the criterium $R_o \geq 20\ \sigma_{RW}^{-1}$.

At time t = 1 nanos ($\Delta t = 0.02$ nanos) we have :

Test	Monte-Carlo	Random Walk	
		$R_o \leq 5\sigma_{RW}$	$R_o \leq 20\sigma_{RW}$
Computer time	3 h 04 mn	6 mn	22 mn
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

Remarks :

1) The Random Walk procedure with $L_o = 0$ and the criterium $R_o \geq 5\ \sigma_{RW}^{-1}$ gave us wrong results : the extrapolation length is essential.

2) Fleck's coefficient ℓ is very small in the opaque medium ($\ell \simeq 5\ 10^{-4}$). Hence it follows that $\tilde{\sigma}_p \simeq \sigma_p$ and $I_* \simeq 1$.

We can see, from figure 7, that the temperature in the opaque zone is the same for the three computations.

CONCLUSION

The diffusion approximation of Fleck's transfer equation given by the multiple scales technique is well satisfied by the numerical tests hence we can use it to construct the Random Walk procedure.

The running time of Fleck's Monte Carlo method can thus be reduced by a factor of 30.

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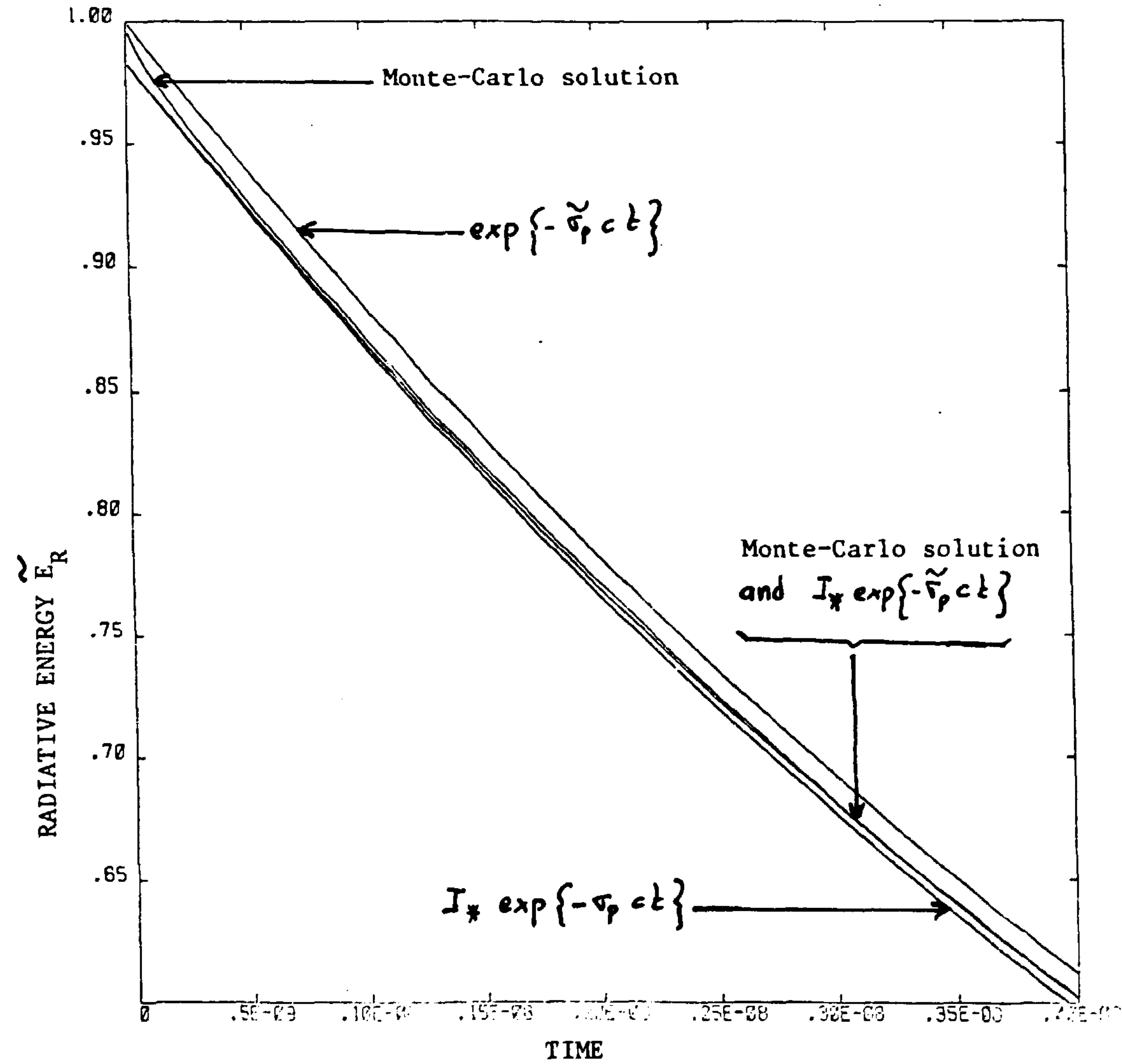
FIGURE 1 - RADIATIVE ENERGY IN R^3



If we assume the domain to be R^3, the expression of the radiative energy simply becomes : $\tilde{E}_R(t) = I_* \exp\{-\tilde{\sigma}_p c t\}$.

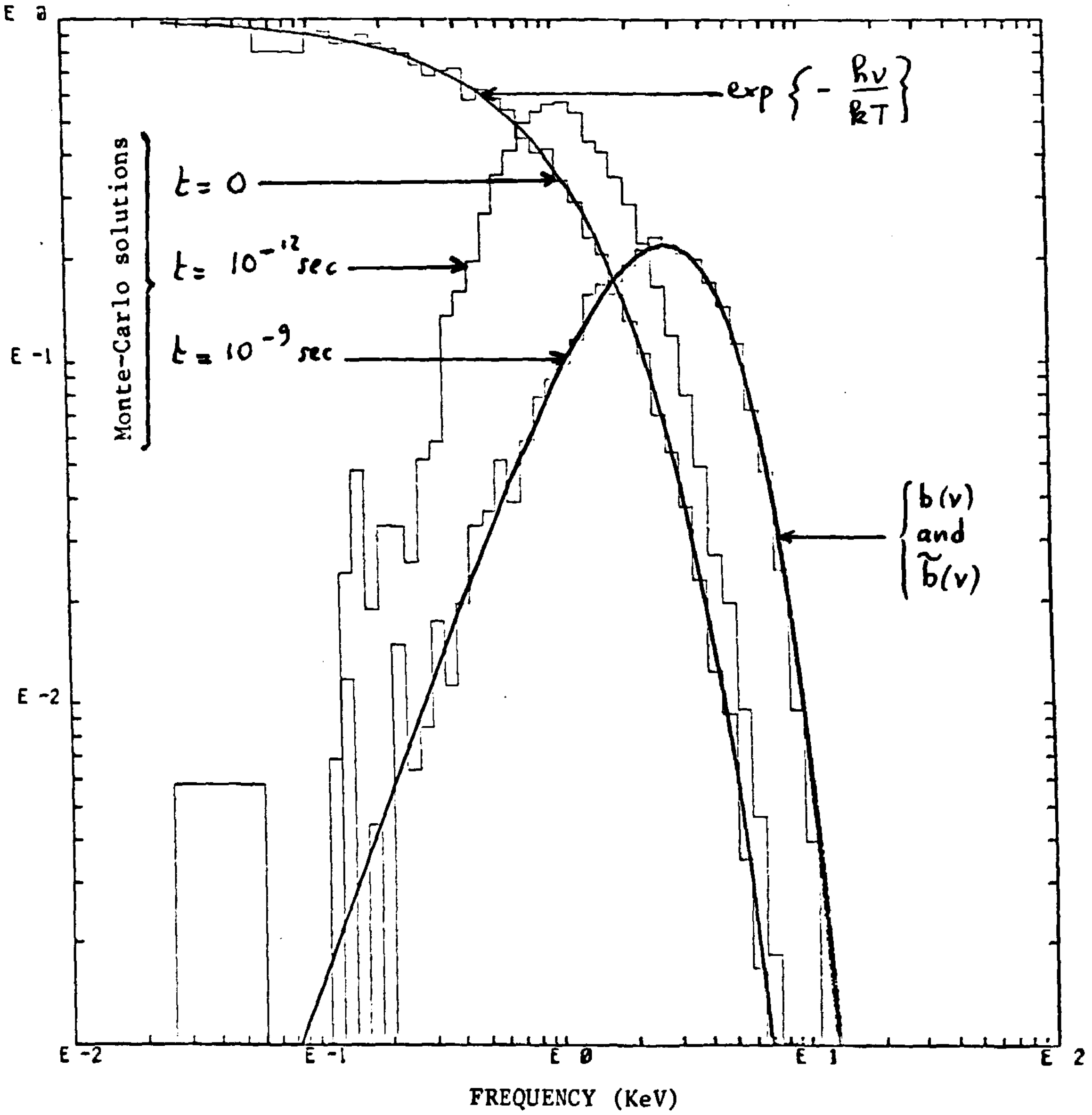
We compare the Monte-Carlo solution of problem (II.1) with $f(\nu) = \frac{k_a(\nu)\, b(\nu)}{k_p}$, $k_a(\nu) = \frac{[illegible]}{\nu^3} \exp\{-\nu/T\}$ (ν and T in Kev) and $\rho = 10^{-3}$, and the diffusion approximation.

We have : $I_* = .9836$, $\sigma_p = 4.163\ 10^{-3}$, $\tilde{\sigma}_p = 4.095\ 10^{-3}$.

We can see that the transport solution is exactly superposed with the diffusion solution $I_* \exp\{-\tilde{\sigma}_p c t\}$

for $t \gg 3\ 10^{-8}$ sec.

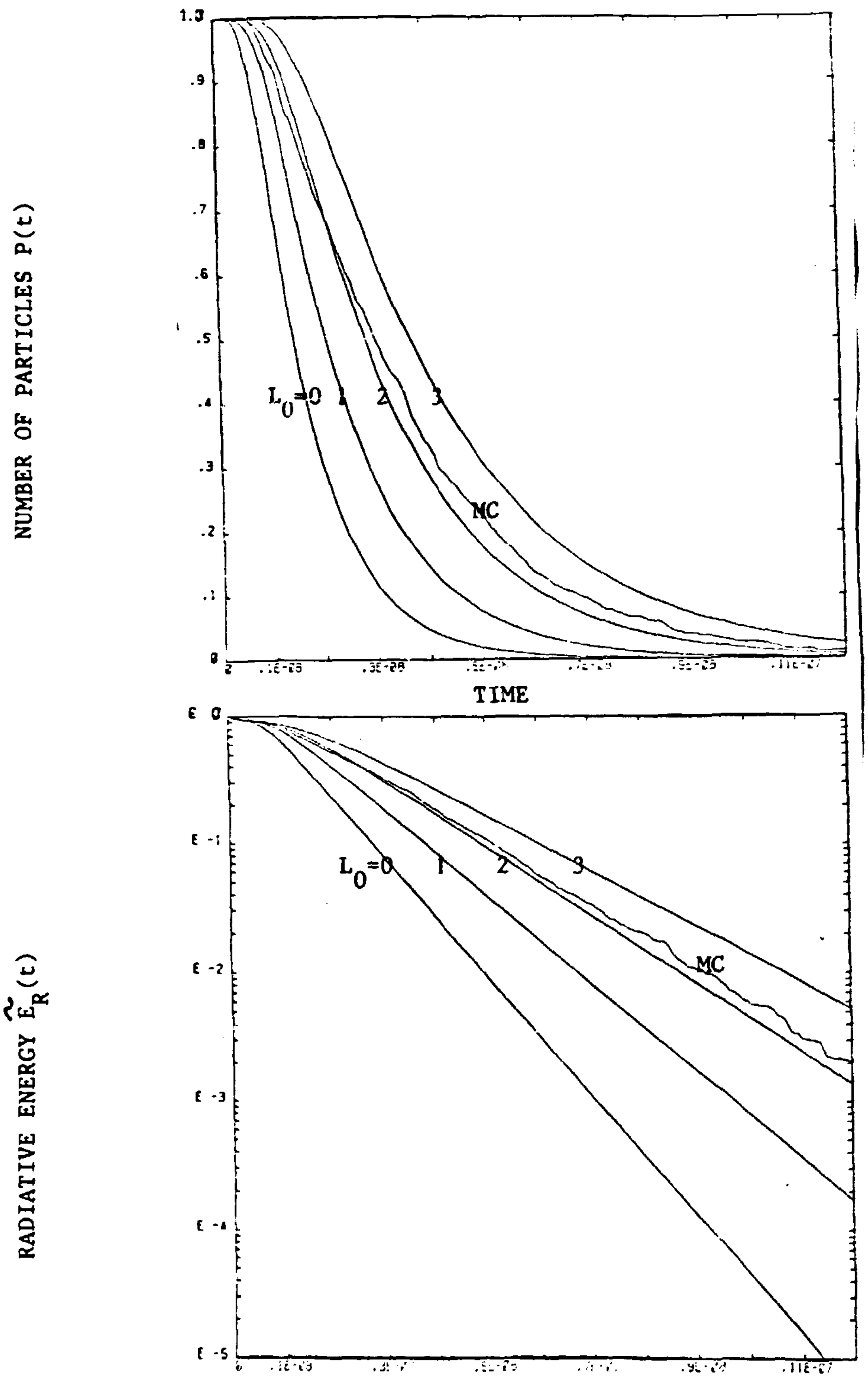
FIGURE 2 - FREQUENCY SPECTRUM



We plot the frequency spectrum, at times $t = 0$, $t = 10^{-12}$ sec. and $t = 10^{-9}$ sec. The parameters are exactly the same as in figure 1 : $D = R^3$, $\rho = 10^{-3}$.

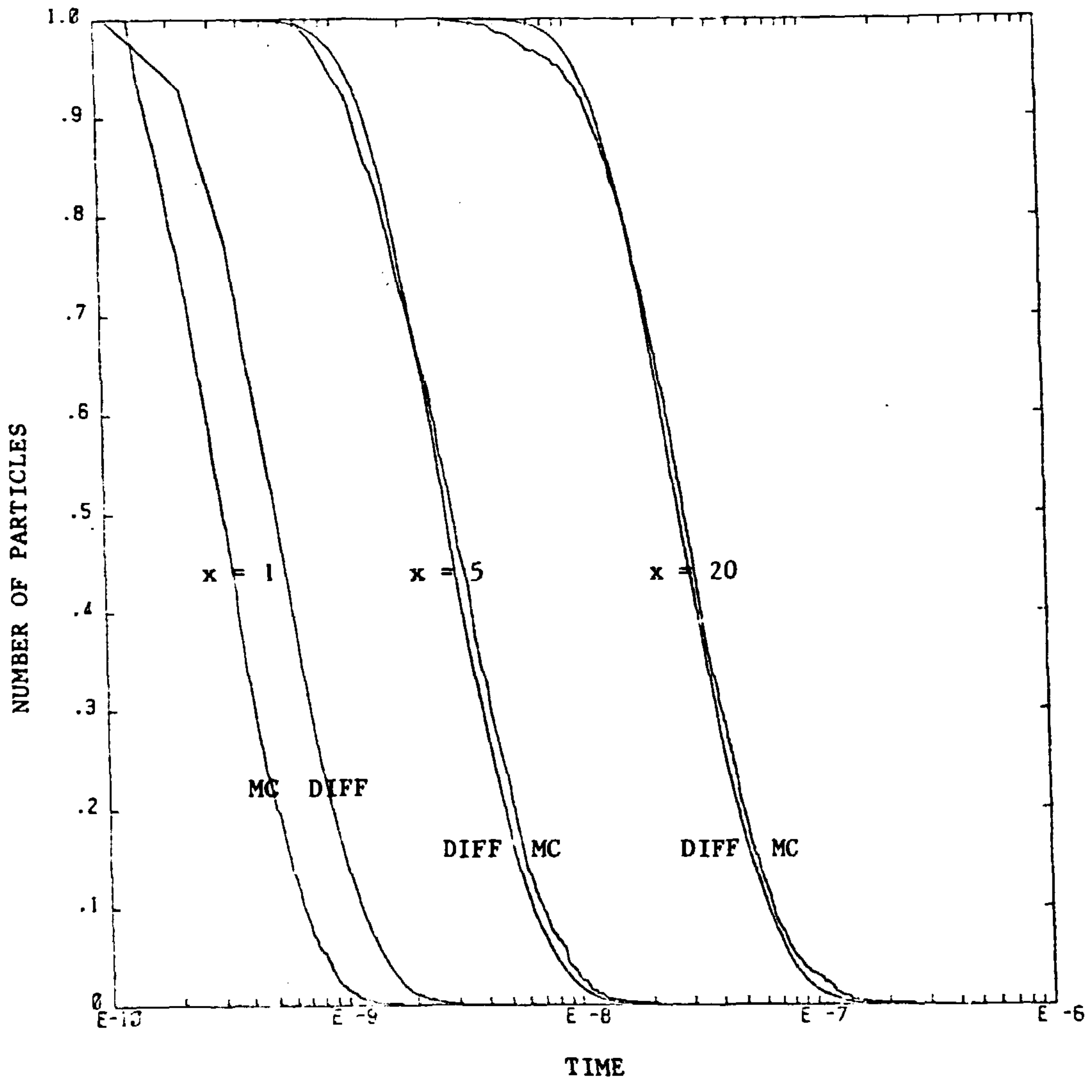
The frequency spectrum is approximately $\tilde{b}(\nu)$ at a very short time.

FIGURE 3 - ESTIMATION OF THE EXTRAPOLATION LENGTH



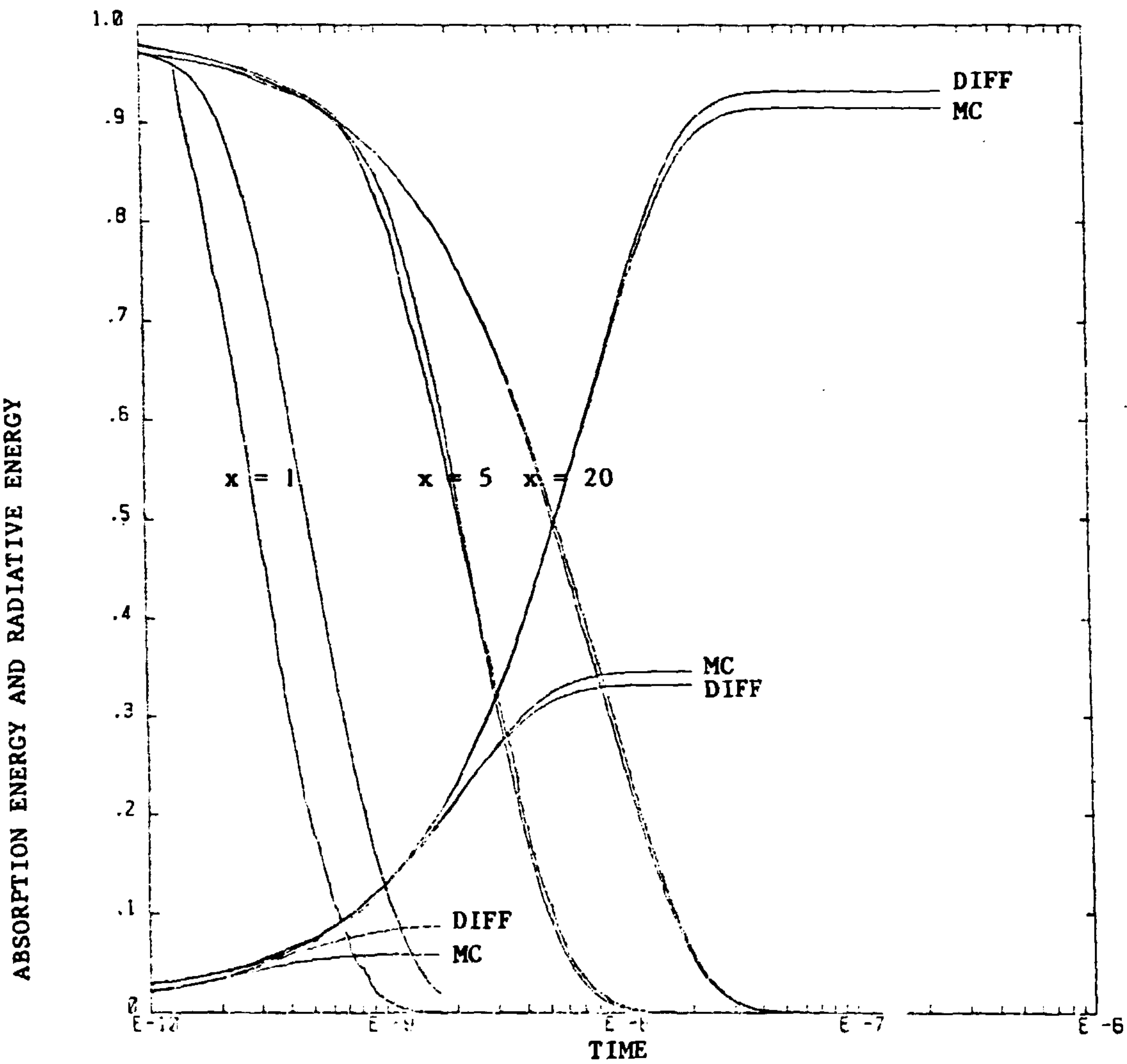
Comparison between Monte-Carlo and diffusion solutions for various values of the extrapolation length L_0 in a sphere of radius $R_o = 5\,\sigma_{Rw}^{-1}$ and $\rho = 10^{-3}$.

FIGURE 4 - DOMAIN OF VALIDITY



Comparison between the Monte-Carlo number of particles in the sphere and the diffusion approximation computed with $L_0 = 2\ \sigma_{R\omega}^{-1}$. The radius of the sphere equals $R_o = x\ \sigma_{R\omega}^{-1}$.

FIGURE 5 - DOMAIN OF VALIDITY

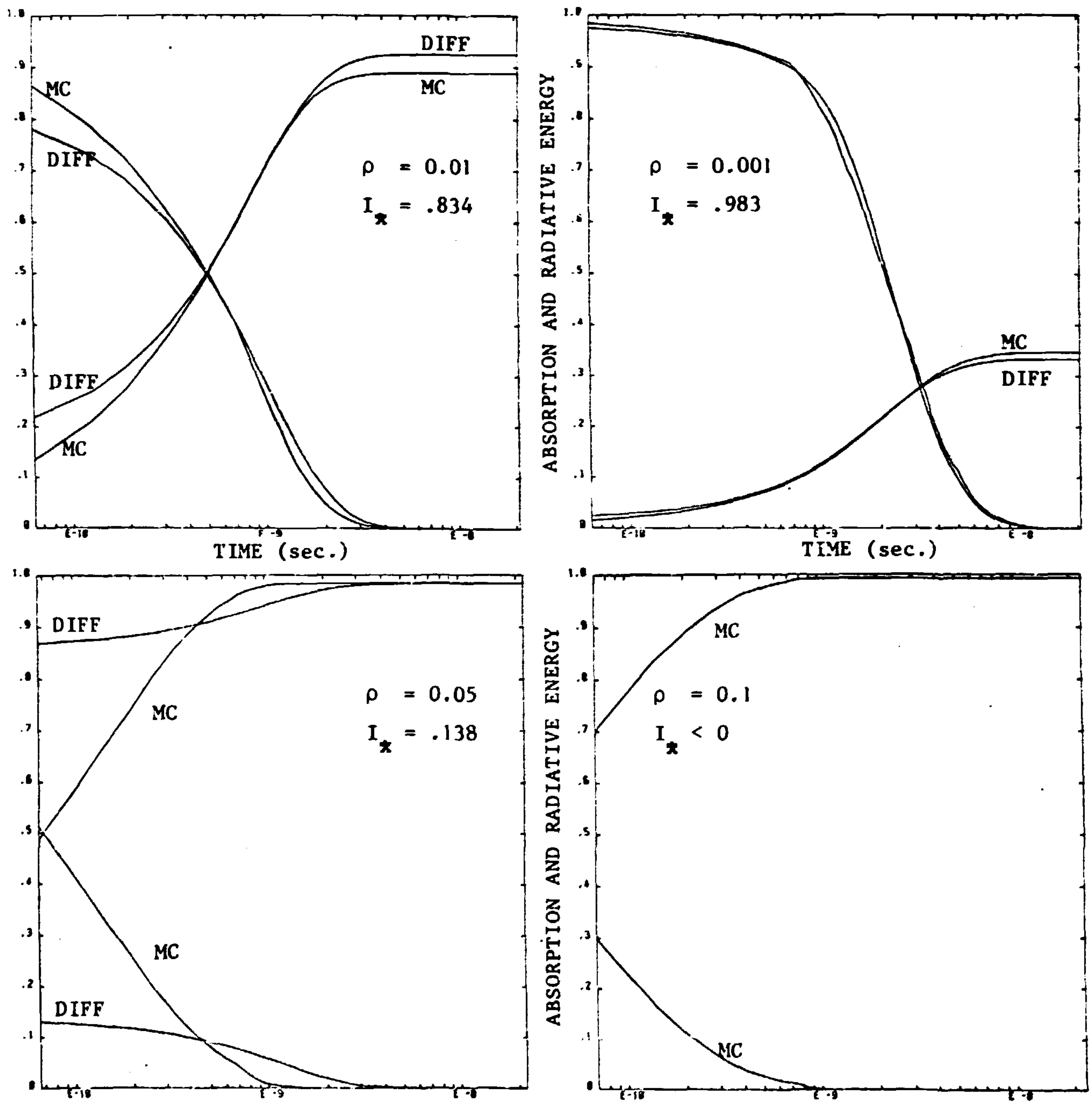


With the same data as for figure 4, we plot the radiative energy $\tilde{E}_R(t) = I_* \exp\{-\tilde{\sigma}_p c t\} P(t)$

and the absorption energy

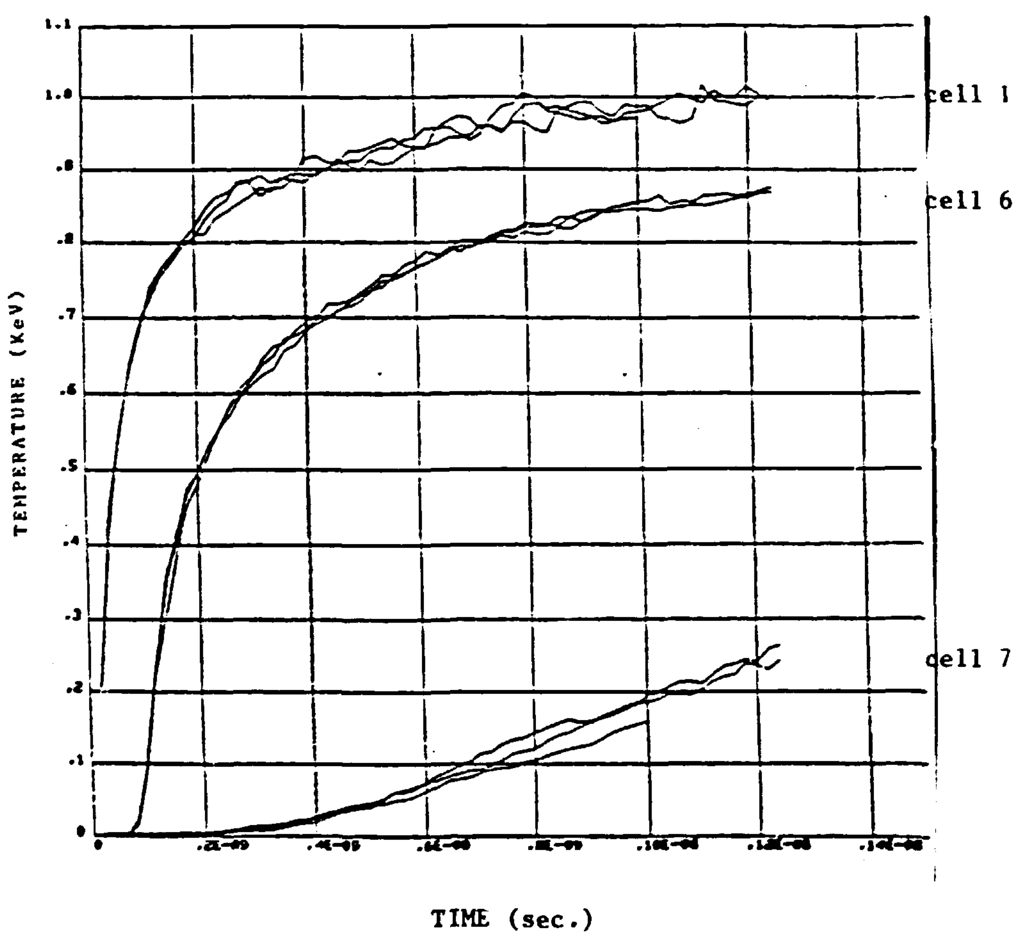
$$\tilde{E}_{abs}(t) = (1 - I_*) + I_* \int_0^t \tilde{\sigma}_p \exp\{-\tilde{\sigma}_p c s\} P(s)\, ds .$$

FIGURE 6 - DOMAIN OF VALIDITY



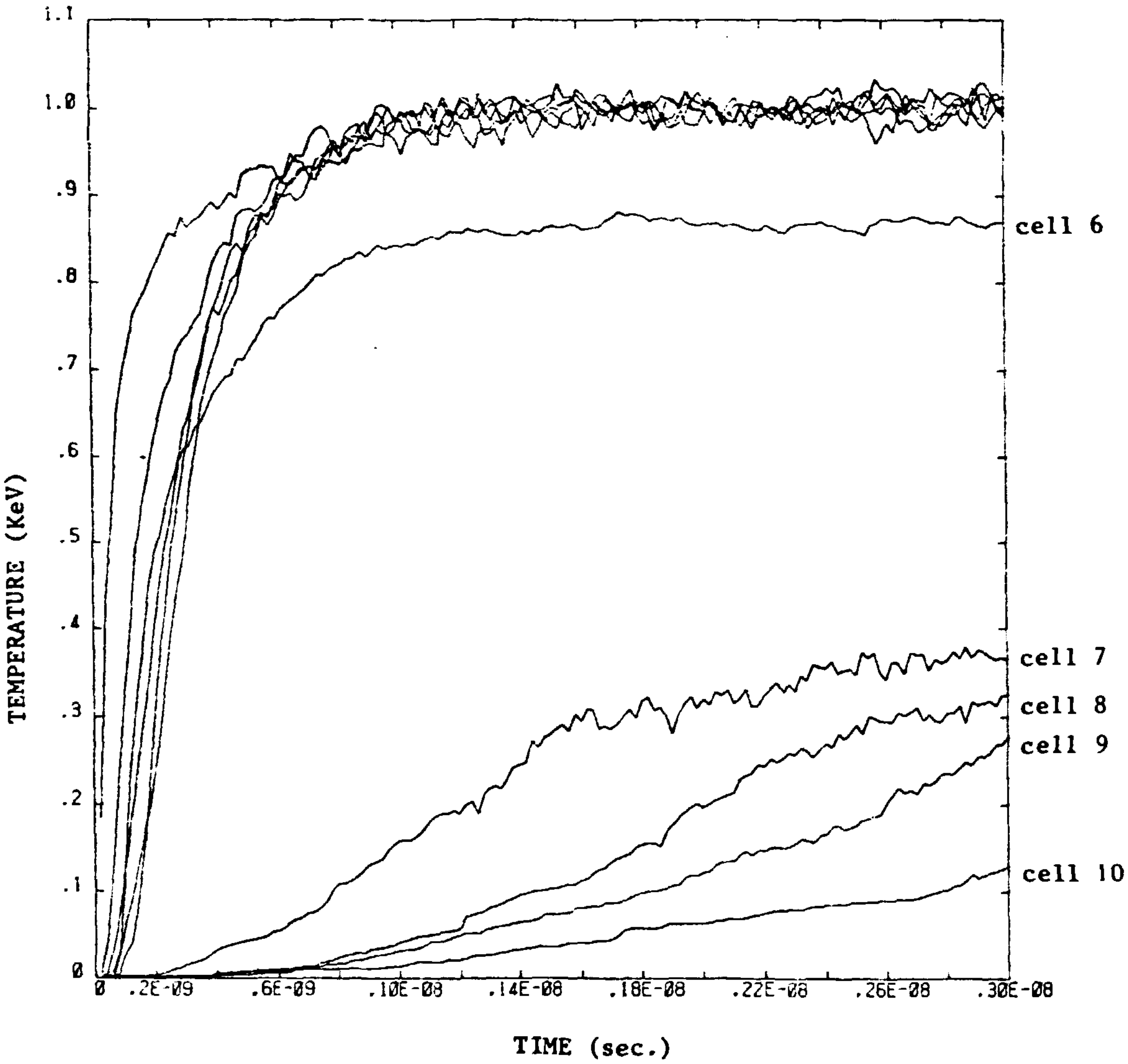
Comparison between the radiative energy and the absorbed energy computed by the Monte-Carlo Method and the diffusion approximation for different values of "ℓ" ($R_o = 5\ \sigma_{R\omega}^{-1}$)

FIGURE 7 - NUMERICAL RESULTS



The temperatures obtained with the three computations (Fleck's Monte-Carlo, Random Walk with $R_0 \leqslant 20\ \sigma_{Rw}^{-1}$ and Random Walk with $R_0 \leqslant 5\sigma_{Rw}^{-1}$) are the same.

FIGURE 8 - BENCHMARK I - Temperatures in the different cells



Data are identical to figure 7 except for the macroscopic cross section : here we use a multigroup description at the frequency spectrun with 50 groups.

FIGURE 9 - BENCHMARK II - Temperature distribution

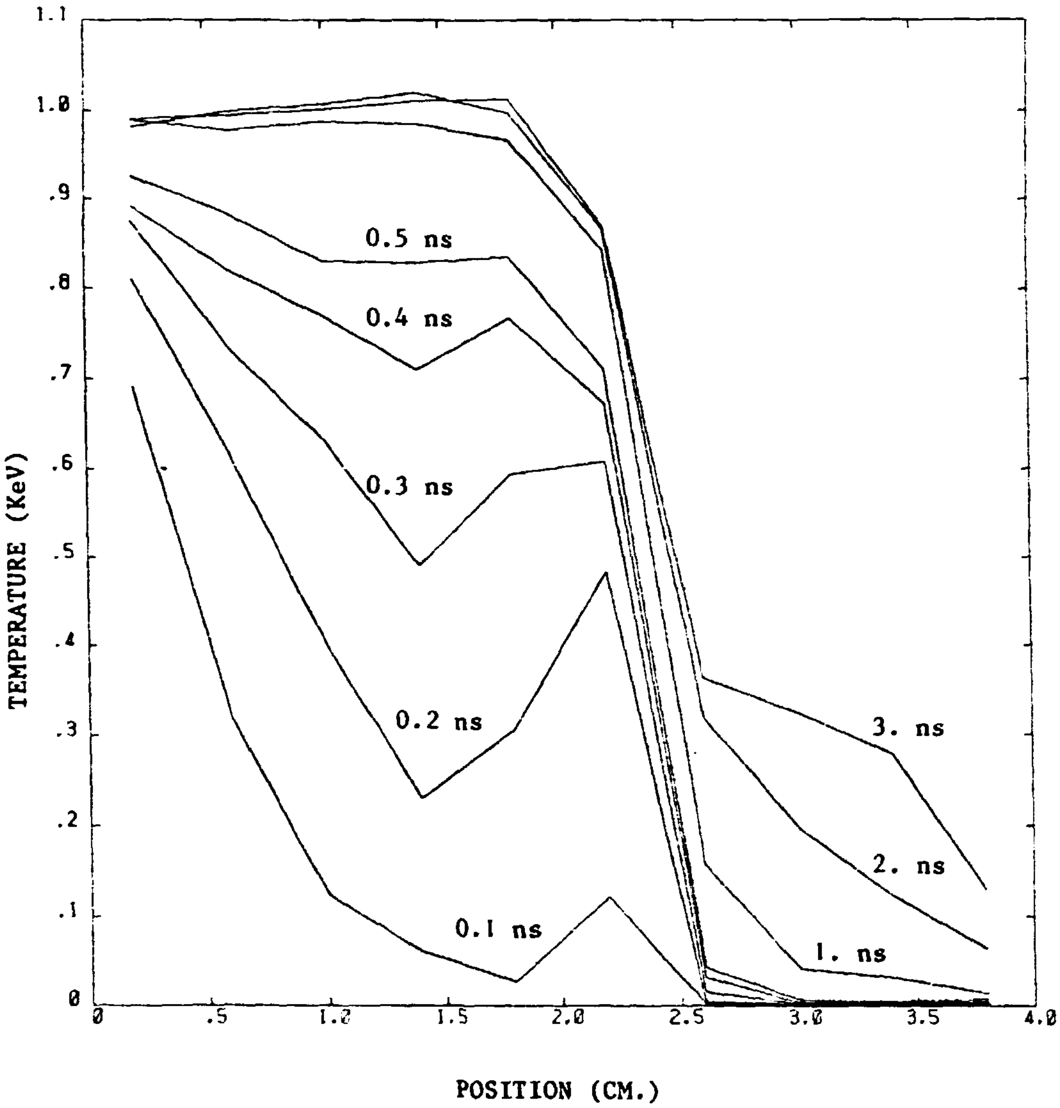
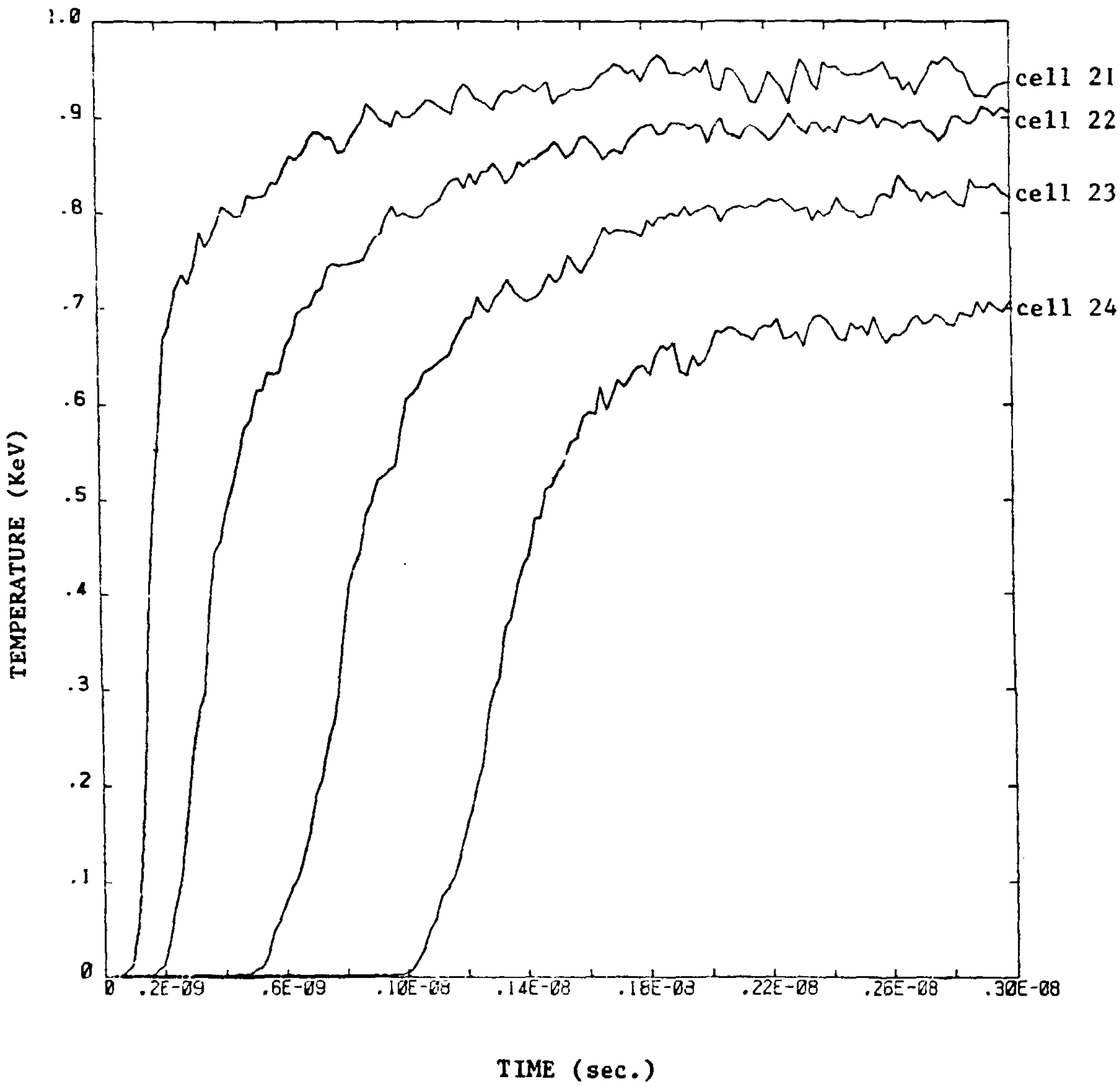


FIGURE 10 - BENCHMARK II - Temperature in the opaque zone



Differences between Benchmark I and II are :

- The incomming flux is linearly increasing between 0 and 10^{-10} sec. and afterwards constant

- There are 40 uniform spatial zones

FIGURE 11 - BENCHMARK II