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**Derivation of the radiative transfer equation  
for scattering media with a spatially varying refractive index.**

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**ABSTRACT:**

We derive in this paper a radiative transfer equation in scattering media with spatially varying refractive index, together with its associated diffusion approximation. We present an approximate result of this diffusion equation in a simple case, and this result is compared to Monte Carlo simulations.

A radiative transfer equation (RTE) in scattering media with a spatially varying refractive index has been derived by H. Ferwerda [1]; T. Khan and H. Jiang [2] deduced the diffusion equation associated to this result. The equation of H. Ferwerda however does not satisfy energy conservation, as can be seen in [2]. In this paper we will reconsider the derivation of the RTE, and will obtain a completely different result. In order to prove the pertinence of our result, we will deduce a diffusion equation from our RTE; we will then obtain an analytical approximate result in the case of low refractive index gradient, for both diffusion equations derived by Khan et al and us. These analytical results are then compared to a Monte Carlo simulation.

The RTE comes from an energy balance in a small cylinder represented on figure 1. Let us consider this energy balance at point  $\vec{r}_0$ , with a direction of propagation parallel to  $\vec{\Omega}_0$  (within the solid angle  $d\Omega$ ). The energy enters to the cylinder at point  $\vec{r}_0$  and at time  $t$ , passing through the elementary area  $dA$ , and it leaves at point  $\vec{r}'$  and at time  $t + dt$ , through  $dA'$ , after a travel  $ds = cdt = c_0 dt / n$  ( $n$  is the varying refractive index). The surface elements  $dA$  and  $dA'$  are chosen to be orthogonal to the rays that are crossing them;  $\vec{\Omega}_0$  is therefore orthogonal to the entry face  $dA$ .

Let us recall the definition of the radiance  $L(\vec{r}_0, \vec{\Omega}_0, t)$ , which is defined so that  $L dA d\Omega \vec{\Omega}_0 \cdot \vec{u}$  is the power flowing within the solid angle  $d\Omega$  through  $dA$  ( $\vec{u}$  is a unit vector orthogonal to  $dA$ ). The energy flow can be materialized by a vector field  $\vec{\Omega}_{\vec{r}_0}(\vec{r}, \vec{\Omega}_0)$ , where  $\vec{\Omega}$  is a unit vector parallel at each point  $\vec{r}$  to the geometrical optical ray passing through this point. The definition of the radiance is a local one, and this vector field has to be considered only at the vicinity of  $\vec{r}_0$ ; if  $\vec{r}$  is a point on the entry face  $dA$ , we can set  $\vec{\Omega}_{\vec{r}_0}(\vec{r}, \vec{\Omega}_0) = \vec{\Omega}_0$ , which means that, in accordance with the definition of  $L$ , we only consider

here the rays that propagate towards the direction  $\vec{\Omega}_0$ . If however  $\vec{r}$  is a point on the ray passing through  $\vec{r}_0$ , at a distance  $ds$  from  $\vec{r}_0$ , we have to use the fundamental equation of geometrical optics [1].

$$\frac{d\Omega^i}{ds} = \frac{1}{n} P_0^{ik} \partial_k n \quad (1)$$

where

$$P_0^{ik} = [\delta^{ik} - \Omega_0^i \Omega_0^k] \quad (2)$$

is the projector on the plane orthogonal to  $\vec{\Omega}_0$  and where we have used the Einstein's summation convention in order to simplify our expressions; we of course have in Euclidean space  $a^i = a_i$ . Let us now find the matrix  $\partial_j \Omega^i$  that links at  $\vec{r} = \vec{r}_0$  an infinitesimal variation  $d\Omega^i$  to an infinitesimal displacement  $dl^j$ . Such a matrix is of course unique, so that one only have to check our solution for every  $dl_{\perp}^j$  that are orthogonal to  $\vec{\Omega}_0$ , and every  $dl_{\parallel}^j$  that are parallel to  $\vec{\Omega}_0$ . This can be readily done for the following derivation rule:

$$\partial_j \Omega^i = \frac{\Omega_{0j}}{n} [\delta^{ik} - \Omega_0^i \Omega_0^k] \partial_k n \quad (3)$$

One indeed have  $\partial_j \Omega^i dl_{\perp}^j = 0$  and  $\partial_j \Omega^i dl_{\parallel}^j = \partial_j \Omega^i \Omega_0^j ds = \frac{d\Omega^i}{ds} ds$ . Let us now write the

energy balance in the cylinder of figure 1, which reads [3]:

$$\begin{aligned} & L(\vec{r}', \vec{\Omega}', t + dt) d\Omega' dA' - L(\vec{r}_0, \vec{\Omega}_0, t) d\Omega dA \\ &= -(\mu_a + \mu_s) ds L(\vec{r}_0, \vec{\Omega}_0, t) d\Omega dA \\ &+ \mu_s ds \int_{4\pi} f(\vec{\Omega}_0, \vec{\omega}) L(\vec{r}_0, \vec{\omega}, t) d\omega d\Omega dA \\ &+ \varepsilon(\vec{r}_0, \vec{\Omega}_0, t) ds d\Omega dA \end{aligned} \quad (4)$$

where  $\mu_a$  is the absorption coefficient per unit length and  $\mu_s$  is the scattering coefficient per unit length.  $f(\vec{\Omega}_0, \vec{\omega})$  is the phase function, which gives the probability for an energy packet traveling in direction  $\vec{\omega}$  to be scattered into direction  $\vec{\Omega}_0$ .  $f$  is normalized according to  $\int_{4\pi} f(\vec{\Omega}_0, \vec{\omega}) d\omega = 1$ . To finish with,  $\varepsilon$  is a source distribution per unit volume and unit solid angle. In order to calculate  $dA'$ , we first notice with H. Ferwerda [1] that we have up to the first order in  $ds, dA$ :

$$\int_{cyl} \partial_i \Omega^i d^3 r = dA' - dA = \partial_i \Omega^i ds dA \quad (5)$$

We get however from (3)  $\partial_i \Omega^i = 0$ , so that  $dA' = dA$ . This point leads to a first difference with the result of H. Ferwerda [1], who has:

$$\partial_i \Omega^i = \sum_i \left[ \frac{1}{n\Omega^i} \partial_i n - \frac{3}{n} \Omega^i \partial_i n \right] \neq 0$$

This expression is however not covariant, as the left member is a scalar and the right one is not ( the term  $1/\Omega^i$  does not transform as a vector so that  $\sum_i \partial_i n / \Omega^i$  is not a scalar): this equation is therefore not preserved through a rotation of the Descartes frame, what leads to difficulties for its physical interpretation. Another difference with the result of H. Ferwerda comes from the solid angle  $d\Omega'$  we take here explicitly into account. Let us introduce 2 vectors  $d\vec{y}_0^{(1)}$  and  $d\vec{y}_0^{(2)}$  orthogonal to  $\vec{\Omega}_0$  and define the solid angle  $d\Omega$  as:

$$d\Omega = \vec{\Omega}_0 \cdot (d\vec{y}_0^{(1)} \times d\vec{y}_0^{(2)}) = \det(\vec{\Omega}_0, d\vec{y}_0^{(1)}, d\vec{y}_0^{(2)}) \quad (6)$$

If  $\vec{\Omega}_0^{(N)} = \vec{\Omega}_0 + d\vec{y}_0^{(N)}$  , we can define the vector field  $\vec{\Omega}^{(N)} = \vec{\Omega}_{\vec{r}_0}(\vec{r}, \vec{\Omega}_0^{(N)})$ . We want the variation of  $\vec{\Omega}^{(N)}$  for an infinitesimal displacement along  $\vec{\Omega}_0^{(N)}$  , that is:

$$\frac{d\vec{\Omega}^{(N)}}{ds} = \vec{\Omega}_0^{(N)} \cdot \vec{\nabla}_{\vec{\Omega}_{\vec{r}_0}}(\vec{r}_0, \vec{\Omega}_0^{(N)})$$

$d\vec{\Omega}^{(N)}/ds$  is a function of  $\vec{\Omega}_0^{(N)}$  that we can develop around  $\vec{\Omega}_0$  :

$$\frac{d\vec{\Omega}^{(N)}}{ds} = \frac{d\vec{\Omega}}{ds} + dy_0^{(N)k} \partial_{\Omega_{0k}} \frac{d\vec{\Omega}}{ds} \quad (7)$$

We can furthermore write:

$$\frac{d\vec{\Omega}^{(N)}}{ds} = \vec{\Omega}_0^{(N)} \cdot \vec{\nabla}_{\vec{\Omega}} + \frac{d}{ds} d\vec{y}^{(N)}$$

As we have already seen that  $d\vec{y}_0^{(N)} \cdot \vec{\nabla}_{\vec{\Omega}} = 0$  , so that  $\vec{\Omega}_0^{(N)} \cdot \vec{\nabla}_{\vec{\Omega}} = \vec{\Omega}_0 \cdot \vec{\nabla}_{\vec{\Omega}} = \frac{d\vec{\Omega}}{ds}$  , we can

therefore conclude:

$$\frac{d}{ds} dy_0^{(N)i} = dy_0^{(N)k} \partial_{\Omega_{0k}} \frac{d\Omega^i}{ds} \quad (8)$$

and

$$d\Omega' = \det \left[ (\Omega_0^i, dy_0^{(1)i}, dy_0^{(2)i}) + ds \left( \frac{d\Omega^i}{ds}, \partial_{\Omega_{0k}} \frac{d\Omega^i}{ds} dy_0^{(1)k}, \partial_{\Omega_{0k}} \frac{d\Omega^i}{ds} dy_0^{(2)k} \right) \right] \quad (9)$$

We will first notice that  $d\vec{\Omega}/ds$  , which is orthogonal to  $\vec{\Omega}_0$  , is in the plane  $(d\vec{y}_0^{(1)}, d\vec{y}_0^{(2)})$  and do not contribute in (9) up to the first order in ds; a second remark is that:

$$P_j^i(\Omega_0^j, dy_0^{(1)j}, dy_0^{(2)j}) = (0, dy_0^{(1)i}, dy_0^{(2)i}) \quad (10)$$

which allows us to write:

$$d\Omega' = \det \left[ \delta_l^i + ds \partial_{\Omega_{0k}} \frac{d\Omega^i}{ds} P_l^k \right] d\Omega = (1 + ds \partial_{\Omega_{0k}} \frac{d\Omega^i}{ds} P_i^k) d\Omega \quad (11)$$

We finally obtain:

$$d\Omega' = (1 - ds \frac{2}{n} \vec{\Omega}_0 \cdot \vec{\nabla} n) d\Omega \quad (12)$$

The derivation of the RTE presents no other difficulties, and following H. Ferwerda [1] we obtain:

$$\begin{aligned} \frac{1}{c} \frac{\partial L}{\partial t} + \vec{\Omega}_0 \cdot \vec{\nabla} L - \frac{2}{n} (\vec{\Omega}_0 \cdot \vec{\nabla} n) L + \frac{1}{n} \vec{\nabla} n \cdot \vec{\nabla}_{\Omega_0} L \\ = -(\mu_a + \mu_s) L + \mu_s \int_{4\pi} f(\vec{\Omega}_0, \vec{\omega}) L(\vec{\omega}) d\omega + \varepsilon \end{aligned} \quad (13)$$

Where we have used, as noticed in [2],  $\vec{\Omega}_0 \cdot \vec{\nabla}_{\Omega_0} L = 0$ . In the following we will drop the subscript 0 and use  $\vec{\Omega}$  instead of  $\vec{\Omega}_0$  in (13). If we integrate now (13) with respect to  $\vec{\Omega}$  over  $4\pi$  sr, if we introduce:

- the average diffuse intensity  $\varphi(\vec{r}, t) = \int_{4\pi} L(\vec{r}, \vec{\Omega}, t) d\Omega$
- the diffuse flux vector  $\vec{j}(\vec{r}, t) = \int_{4\pi} L(\vec{r}, \vec{\Omega}, t) \vec{\Omega} d\Omega$
- the source term  $E(\vec{r}, t) = \int_{4\pi} \varepsilon(\vec{r}, \vec{\Omega}, t) d\Omega$

and if we notice with Khan et al [2] that  $\int_{4\pi} \vec{\nabla}_{\Omega} L d\Omega = 2\vec{j}$ , we directly obtain from (13) the

conservation equation:

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} + \vec{\nabla} \cdot \vec{j} + \mu_a \varphi = E \quad (14)$$

This equation warrant the conservation of the energy density  $W = \varphi / c$ , which was not the case with the equation of H. Ferwerda (see [2]) and is a first point that validate the RTE derived in this paper. Let us now derive a diffusion equation from (13), in order to perform

some comparisons with Monte Carlo simulations. The diffusion approximation consists in setting [2,3]:

$$I(\vec{r}, \Omega, t) = \frac{1}{4\pi} \varphi(\vec{r}, t) + \frac{3}{4\pi} \vec{j}(\vec{r}, t) \cdot \vec{\Omega} \quad (15)$$

Let us insert (15) in (13), multiply by  $\vec{\Omega}$  and integrate with respect to  $\vec{\Omega}$ . An integral of a product of an odd number of  $\vec{\Omega}$  components, like  $\int_{4\pi} \vec{\Omega} d\Omega$  or  $\int_{4\pi} \Omega^i \Omega^j \Omega^k d\Omega$ , is null for obvious symmetry arguments. We furthermore have the well-known relations [3]:

$$\int_{4\pi} \Omega^i \Omega^j d\Omega = \frac{4\pi}{3} \delta^{ij}$$

and

$$\frac{1}{4\pi} \int_{4\pi} f(\vec{\Omega}, \vec{\omega}) \Omega^i \omega^j d\Omega d\omega = \frac{g}{3} \delta^{ij}$$

where  $g = \frac{1}{4\pi} \int_{4\pi} f(\vec{\Omega}, \vec{\omega}) \vec{\Omega} \cdot \vec{\omega} d\Omega d\omega$  is the anisotropy factor. From these relations we obtain:

$$\frac{1}{c} \frac{\partial \vec{j}}{\partial t} + \frac{1}{3} \vec{\nabla} \varphi - \frac{2}{3n} \vec{\nabla} n \varphi = -[\mu_a + (1-g)\mu_s] \vec{j} + F$$

where  $\vec{F}(\vec{r}, t) = \int_{4\pi} \varepsilon(\vec{r}, \vec{\Omega}, t) \vec{\Omega} d\Omega$ . Assuming  $\frac{\partial \vec{j}}{\partial t} = \vec{0}$  leads to the modified Fick law:

$$\vec{j} = -D \vec{\nabla} \varphi + \frac{2D}{n} \vec{\nabla} n \varphi + 3D \vec{F} \quad (16)$$

The diffusion equation comes from the insertion of (16) in the conservation equation (14):

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} - \vec{\nabla} \cdot [D \vec{\nabla} \varphi] + 2 \vec{\nabla} \cdot \left[ \frac{D}{n} \vec{\nabla} n \varphi \right] + \mu_a \varphi = E - 3 \vec{\nabla} \cdot [D \vec{F}] \quad (17)$$

which has to be compared to the diffusion equation obtained by Khan et al [2] from the result of H. Ferwerda [1]:

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} - \vec{\nabla} \cdot [D \vec{\nabla} \varphi] - \frac{2D}{n} \vec{\nabla} n \cdot \vec{\nabla} \varphi + \mu_a \varphi = E - \frac{6D}{n} \vec{\nabla} n \cdot \vec{F} - 3 \vec{\nabla} \cdot [D \vec{F}] \quad (18)$$

If we consider now the simple case with  $\mu_a = 0$ ,  $D$  constant,  $n = n_0 + \vec{q} \cdot \vec{r}$  with constant  $\vec{q}$ , and with an isotropic point-like source ( $E = \delta(\vec{r})\delta(t)$ ,  $\vec{F} = \vec{0}$ ), we obtain for equation (17):

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} - D \Delta \varphi + \frac{2D}{n} \vec{q} \cdot \vec{\nabla} \varphi - \frac{2D}{n^2} q^2 \varphi = \delta(\vec{r}) \delta(t) \quad (19)$$

and for equation (18):

$$\frac{1}{c} \frac{\partial \varphi}{\partial t} - D \Delta \varphi - \frac{2D}{n} \vec{q} \cdot \vec{\nabla} \varphi = \delta(\vec{r}) \delta(t) \quad (20)$$

The leading difference between (19) and (20) is therefore the sign of the term  $\vec{q} \cdot \vec{\nabla} \varphi$ .

Let us search a solution of (19) of the form:

$$\varphi = A t^{-\frac{3}{2}} \exp \left[ -\frac{r^2}{4Dct} + y \right] \quad (21)$$

If we assume that  $y$  is of the same order than  $q$ , and if we neglect the second order terms, inserting (21) in (19) for  $t > 0$  leads to:

$$\frac{1}{c} \frac{\partial y}{\partial t} - D \Delta y + \frac{\vec{r} \cdot \vec{\nabla} y}{ct} - \frac{r^2 \vec{r} \cdot \vec{q}}{4nD(ct)^2} = 0 \quad (22)$$

and we find:

$$y = \frac{1}{2n} \left[ \frac{r^2}{4Dct} + \frac{5}{2} \right] \vec{q} \cdot \vec{r} \quad (23)$$

The coefficient A in (21) is obtained by comparison, in the limit  $t \rightarrow 0$ , to the classical result without variation of the refractive index [4]:

$$A = \frac{c_0}{n_0} (4\pi D c_0 / n_0)^{-3/2} \quad (24)$$

Concerning equation (20) the substitution (21) leads to:

$$\frac{1}{c} \frac{\partial y}{\partial t} - D \Delta y + \frac{\vec{r} \cdot \vec{\nabla} y}{ct} + 2 \frac{\vec{r} \cdot \vec{q}}{nct} - \frac{r^2 \vec{r} \cdot \vec{q}}{4nD(ct)^2} = 0 \quad (25)$$

that is:

$$y = \frac{1}{2n} \left[ \frac{r^2}{4Dct} - \frac{3}{2} \right] \vec{q} \cdot \vec{r} \quad (26)$$

with of course the same value for A.

Let us now compare these results with Monte Carlo simulations [5]. We stress here on the fact that Monte Carlo simulations are based on the propagation of multiple random walkers that propagate on optical rays and experience absorption and scattering events: These simulations are therefore completely disconnected from the RTE, and can be used to discriminate all the results presented here. We simulate a scattering medium with  $\mu_a = 0$ ,  $\mu_s = 50 \text{ cm}^{-1}$ , an Henyey-Greenstein phase function with an anisotropy factor  $g = 0.8$ , and a refractive index  $n = n_0 + qz$  with  $n_0 = 1.5$  and  $q = 0.02 \text{ cm}^{-1}$ . The average diffuse intensity obtained from these simulations is presented in figure 2 for a point located on the z axis at  $z = 2 \text{ cm}$ . The noisy curve comes from the Monte Carlo simulations, and the bold line corresponds to our result (equations (21,23,24)). The result obtained from the work of H.

Ferwerda (equations (21,24,26) ) is presented with dashed line, and the dotted line in the middle of the three curves is the average diffuse intensity  $\varphi_0$  without refractive index gradient, that is with  $q = 0$  . As can be seen in this figure, there is a fundamental difference between our result and the result of H. Ferwerda, as H. Ferwerda predicts a decrease of the average diffuse intensity when we predict an increase of this quantity, in accordance with Monte Carlo simulations. This point is more striking in figure 3, where we plot the quantities  $(\varphi - \varphi_0)/\varphi_0$  corresponding to the curves of figure 2. In fact the equation of geometrical optics (1) predicts that the rays are deviated toward the direction of increasing refractive index values, so one should intuitively await an increase of the diffuse intensity in the direction of the refractive index gradient. Our result presents a very satisfying correspondence with Monte Carlo simulation. We recall that it is obtained without any adjustable parameter. We present in figure 4 and 5 the same results for  $z = -2cm$  , with the same conclusions.

As a conclusion, we derived a radiative transfer equation in scattering media with spatially varying refractive index, together with a diffusion approximation solved in a simple case. Our results are in very good correspondence with Monte Carlo simulations.

## References

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## Figure Captions

### Figure 1:

Cylinder on which the energy balance is considered. The vector field  $\vec{\Omega}$  is parallel at each point  $\vec{r}$  to the geometrical optical ray passing through this point.

### Figure 2:

Average diffuse intensity for  $z = 2\text{cm}$ . The noisy curve comes from the Monte Carlo simulations and the bold line corresponds to our result. The result obtained from the work of H. Ferwerda is presented with dashed line, and the dotted line in the middle of the three curves corresponds to the case  $q = 0$ .

### Figure 3:

$(\varphi - \varphi_0) / \varphi_0$  for  $z = 2\text{cm}$ . The noisy curve comes from the Monte Carlo simulations and the bold line corresponds to our result. The result obtained from the work of H. Ferwerda is presented with dashed line.

### Figure 4:

Average diffuse intensity for  $z = -2\text{cm}$ . The noisy curve comes from the Monte Carlo simulations, and the bold line corresponds to our result. The result obtained from the work of H. Ferwerda is presented with dashed line, and the dotted line in the middle of the three curves corresponds to the case  $q = 0$ .

**Figure 5:**

$(\varphi - \varphi_0) / \varphi_0$  for  $z = -2cm$ . The noisy curve comes from the Monte Carlo simulations and the bold line corresponds to our result. The result obtained from the work of H. Ferwerda is presented with dashed line.

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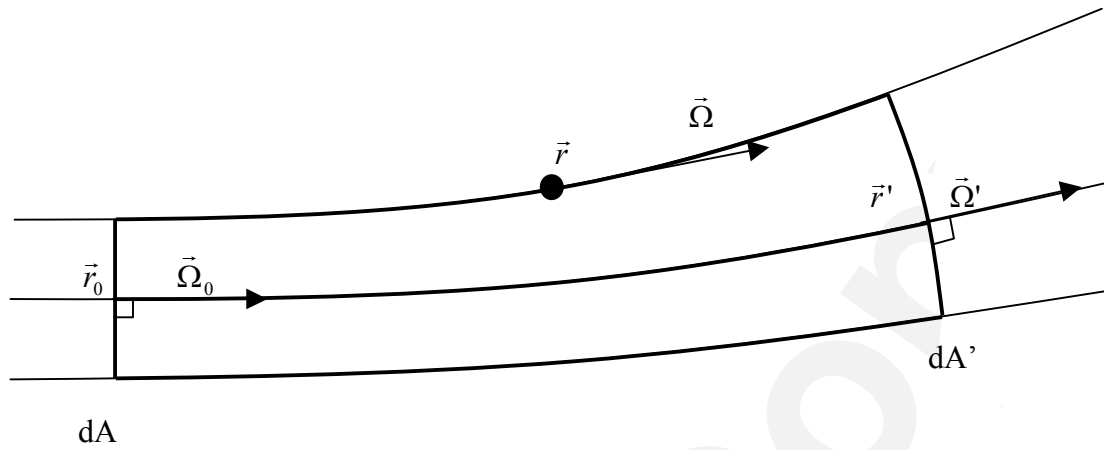


Figure 1

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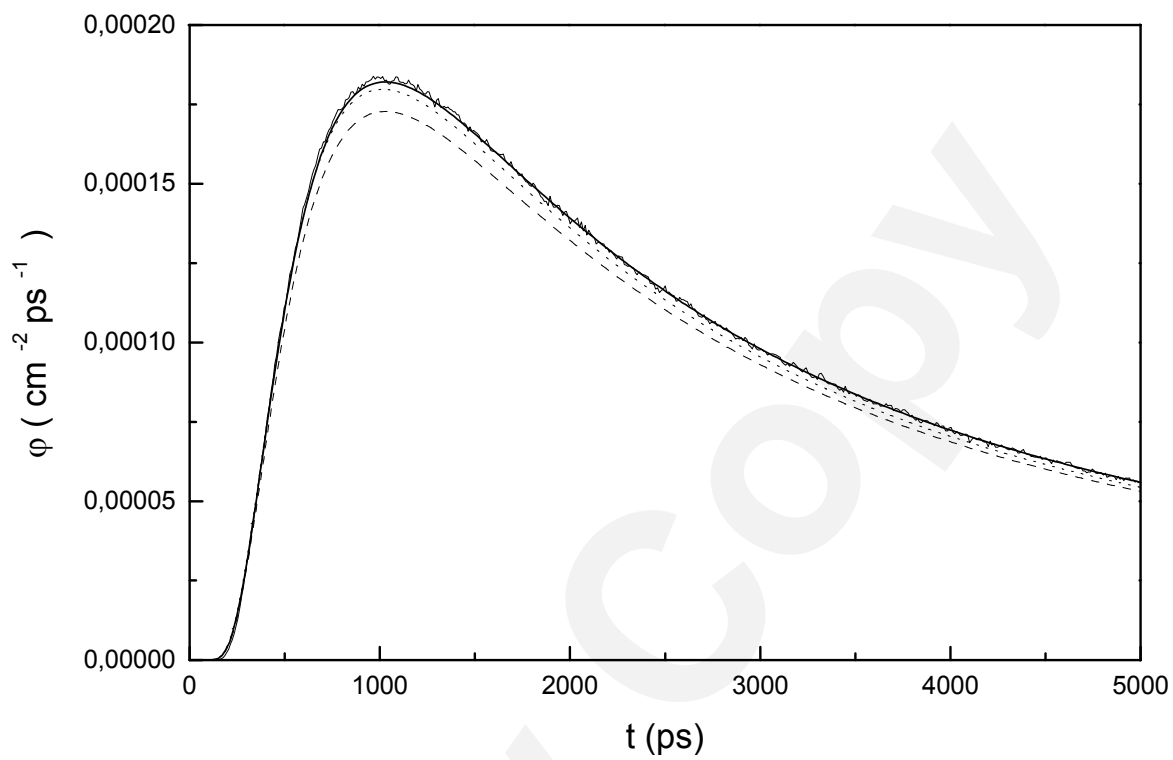


Figure 2

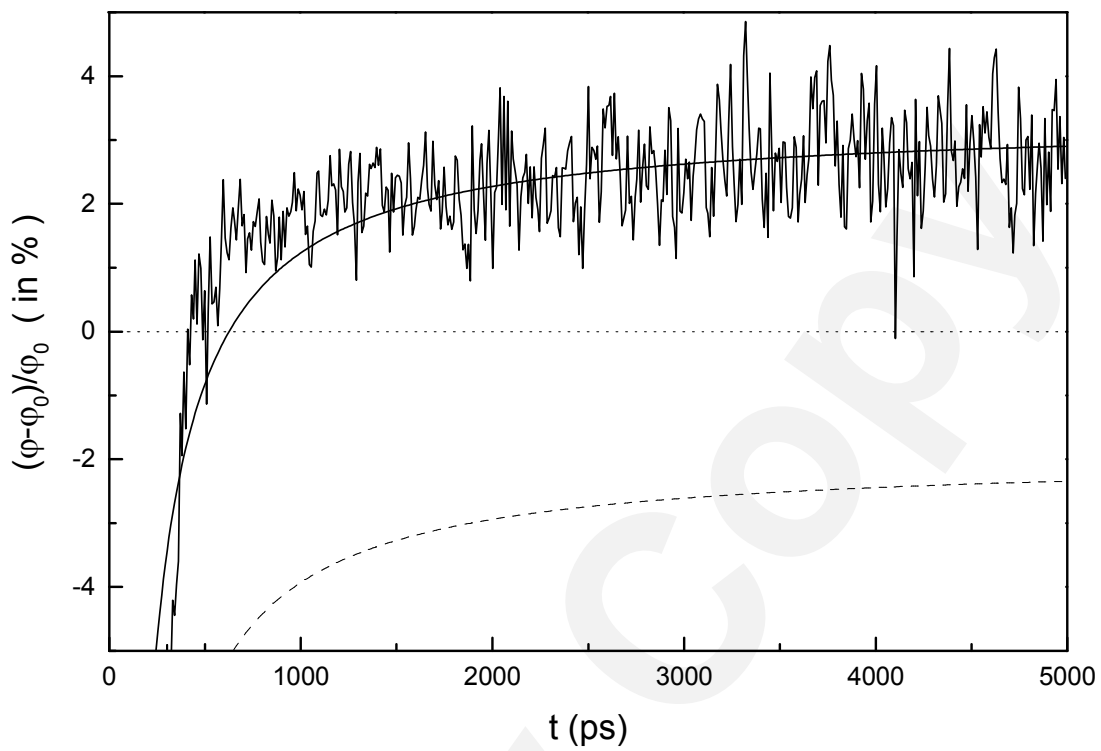


Figure 3

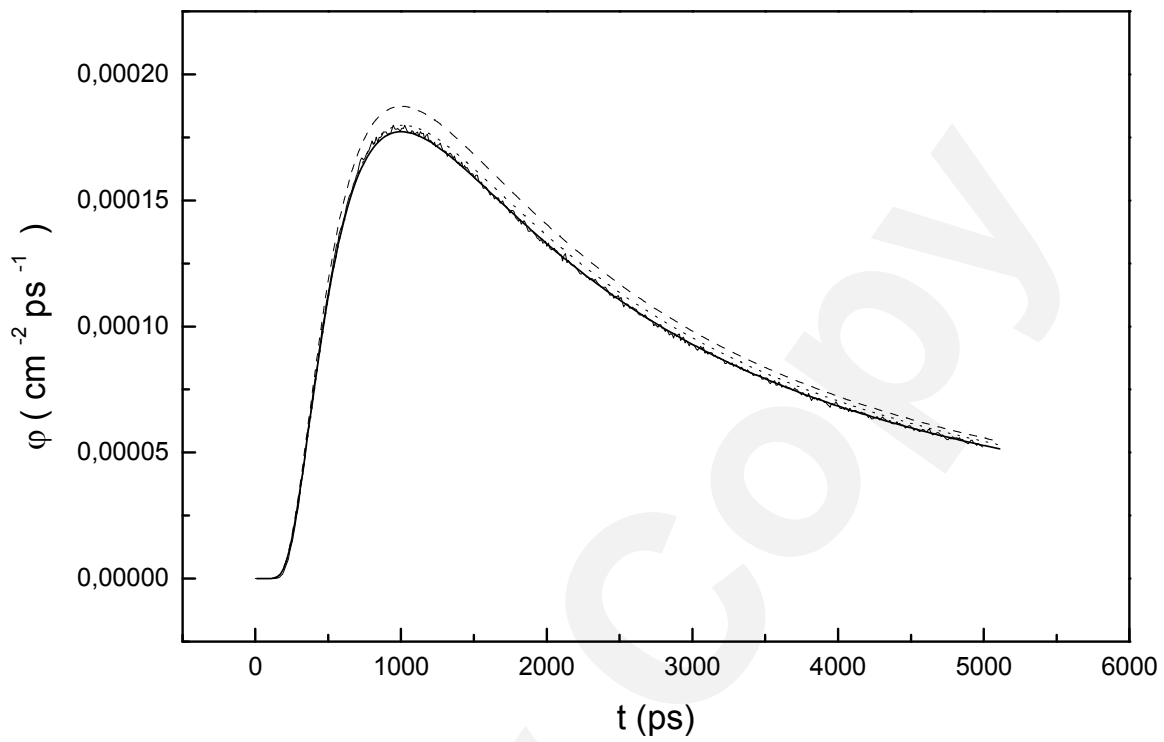


Figure 4

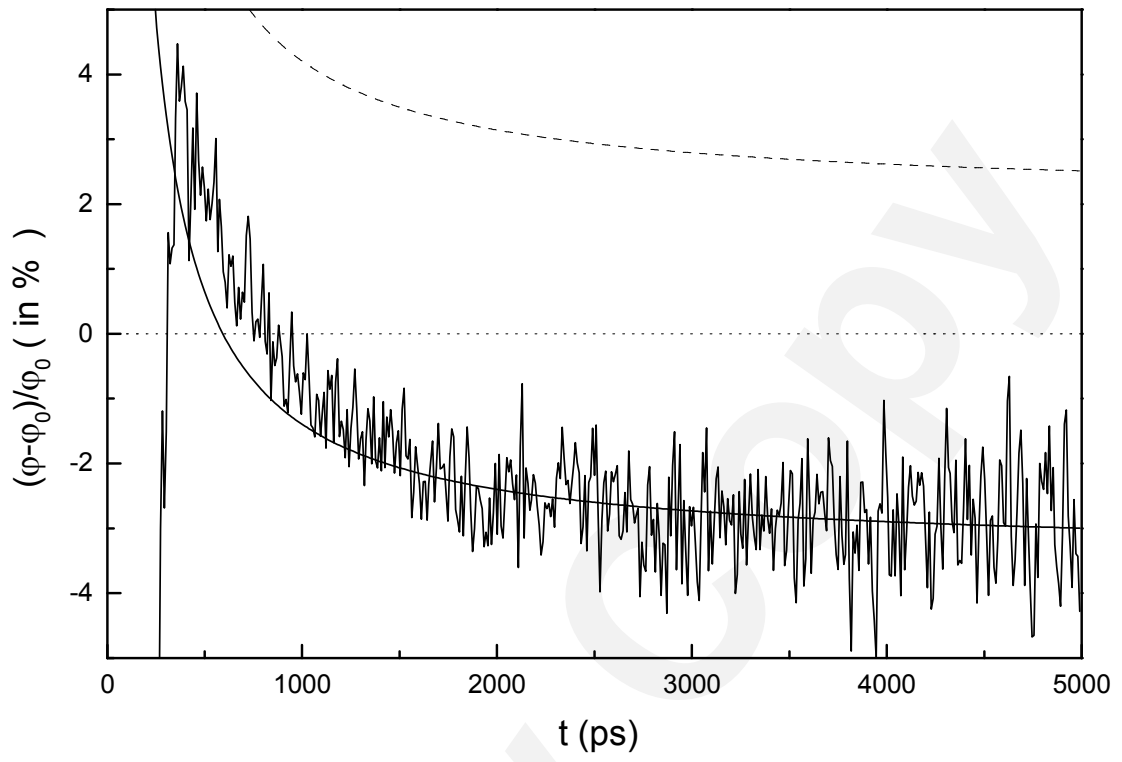


Figure 5