

# Primary and scattering contributions to beta scaled dose point kernels by means of Monte Carlo simulations

## Contribuições primária e espalhada para dosimetria beta calculadas pelo dose point kernels empregando simulações pelo Método Monte Carlo

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### Abstract

Beta-emitters have proved to be appropriate for radioimmunotherapy. The dosimetric characterization of each radionuclide has to be carefully investigated. One usual and practical dosimetric approach is the calculation of dose distribution from a unit point source emitting particles according to any radionuclide of interest, which is known as dose point kernel. Absorbed dose distributions are due to primary and radiation scattering contributions. This work presented a method capable of performing dose distributions for nuclear medicine dosimetry by means of Monte Carlo methods. Dedicated subroutines have been developed in order to separately compute primary and scattering contributions to the total absorbed dose, performing particle transport up to 1 keV or least. Preliminarily, the suitability of the calculation method has been satisfactory, being tested for monoenergetic sources, and it was further applied to the characterization of different beta-minus radionuclides of nuclear medicine interests for radioimmunotherapy.

**Keywords:** nuclear medicine, beta-emitter, dose point kernel, Monte Carlo simulation.

### Resumo

Fontes de radiação que emitem partículas beta são comprovadamente apropriadas para radioimunoterapia. Para tanto, a caracterização dosimétrica do respectivo radionuclídeo tem de ser realizada cuidadosamente. Uma abordagem dosimétrica prática e usual é o cálculo da distribuição de dose de uma fonte pontual unitária emitindo partículas de acordo com o radionuclídeo de interesse, a qual é conhecida como *dose point kernel*. As distribuições de doses absorvidas são devidas às contribuições das radiações primária e espalhada. Este estudo apresenta um método capaz de verificar as distribuições de dose para dosimetria em medicina nuclear empregando o método Monte Carlo. Subrotinas têm sido desenvolvidas para permitir calcular separadamente as contribuições primária e espalhada da dose absorvida total, utilizando o transporte de partículas até 1keV ou menos. Preliminarmente, a adequação do método de cálculo foi testada de forma satisfatória para fontes monoenergéticas, e foi ainda aplicada à caracterização de diferentes radionuclídeos beta emissores de interesse em medicina nuclear para radioimunoterapia.

**Palavras-chave:** medicina nuclear, beta emissor, *dose point kernel*, simulação Monte Carlo.

### Introduction

The interest from the nuclear medicine community in developing novel radiopharmaceuticals for radioimmunotherapy motivates active investigations devoted to the study and application of radiolabeled molecules with the capability for selectively distinguish treatment target and further tumor cells irradiation. The utilization of this kind of pharmaceuticals results in spatial activity distributions with extremely non-uniform characteristics

within the patient. Actually, this feature constitutes precisely the main advantage of these methods in view of maximizing the discrimination between affected and healthy tissue<sup>1</sup>.

Activity distribution may be determined by means of different modalities. Nowadays, it is mainly measured using modern imaging techniques but it is also possible to infer it by semi-empirical methods. The information about the activity distribution is then incorporated in the treatment planning system in order to obtain an estimation of the corresponding dose distribution. In

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this sense, patient-specific dose distribution may be attained by suitable calculations starting from activity distribution by means of either Monte Carlo simulation or direct analytical methods<sup>1,2</sup>.

The dose distribution about a unit point source of any radio-nuclide of interest — known as dose point kernel (DPK) — has proven to be a particularly useful tool for dosimetric calculation by means of analytical methods<sup>3,4</sup>. Analytical procedures, however, can be straightforwardly performed only when considering homogeneous media. Therefore, analytical procedures may show non-negligible limitations for practical situations.

This work presented a method capable of calculating DPK for nuclear medicine dosimetry by means of Monte Carlo methods. In addition, dedicated subroutines have been developed in order to compute primary and scattering contributions to the total absorbed dose. The developed calculation method has been applied to the characterization of different beta-minus radionuclides of interest for nuclear medicine therapy.

## Materials and methods

### Theoretical background

The starting point for the proposed method is to consider a simple situation of an isotropic point source emitting electrons moving radially outward. Boltzmann radiation transport equation along with the continuous slowing down approximation (CSDA) for charged particles predict that emitted electrons shall continuously slow down according to the stopping power function  $S(E)$ , which depends on the electron kinetic energy and, of course, physical properties of the irradiated material.

For a monoenergetic source, which energy is  $E_0$ , it can be calculated the remaining energy  $E(s)$  at a distance  $s$  from the source location by means of:

$$\int_{E(s)}^{E_0} \frac{dE}{S(E)} = s \quad (1)$$

where  $S(E)$  is the stopping power.

For practical reasons, it is usually convenient to introduce the scaled DPK for beta particles ( $F$ ) by means of the following definition:

$$F(s/R_{CSDA}) = \frac{\delta E(s)/E_0}{\delta s/R_{CSDA}} \quad (2)$$

where  $\delta s$  stands for the shell thickness,  $R_{CSDA}$  is the particle range in the CSDA,  $\delta E(s)$  is energy delivered in the shell between  $s$  and  $s + \delta s$ .

In order to avoid a singularity at the origin, it is assumed by convention that  $F(s=0)$  equals  $R_{CSDA}/40$ , where  $R_{CSDA}$  represents the CSDA range defined by:

$$R_{CSDA} = \int_0^{E_0} \frac{dE}{S(E)} \quad (3)$$

Analytical approaches for solving the presented model need to assume implicitly some approximations. Specifically, straight-line motion along with continuous energy loss have been taken as valid for electron interaction mechanism. However, it is actually known that departures from continuous slowing down arise from multiple scattering and energy loss fluctuations, like delta-ray and Bremsstrahlung production.

Contrary to analytical techniques, Monte Carlo calculations of DPK are capable of more realistic approaches, mainly due to the possibility of handling multiple scattering as well as radiative energy losses. In this framework, it becomes possible to consider the fact that some part of the energy loss straggling may be carried out to positions far away, even at distances larger than  $R_{CSDA}$ .

When considering non monoenergetic sources, like radio-nuclides, it is necessary to calculate scaled DPK obtained by weighting the corresponding associated spectra. This aim is usually attained decomposing the spectrum into  $M$  groups according to the branching probability  $b_i$  and end-point energy  $E_i$ , as follows:

$$N(E) = \sum_{i=1}^M p_i N_i(E) \quad (4)$$

where  $N$  indicates the channel intensity.

### Implemented calculation method

Specific subroutine has been developed based on the PENELOPE v. 2008 main code<sup>5</sup> to calculate scaled DPK. The subroutine has been specifically developed for assessing primary and scattering contributions. The primary component is considered as dose contributions from primary particles, which are actually emitted by the point source. On the other hand, the scattering component is due to all kind of dose contributions that carry out when scattered (secondaries etc.) particles deposit energy within the shell. When considering electrons as primary particles, the implemented interaction mechanisms that may change particle phase state and/or generate secondary radiation were soft event (energy and angle variations lower than specific threshold values), elastic collision, hard inelastic collision, Bremsstrahlung emission, inner-shell (K, L and M) impact ionization and delta interaction.

Scaled DPK were simulated considering a 10 cm radius water-equivalent spherical phantom and energy deposition was tallied in concentric shells having thickness of  $R_{CSDA}/40$ , where the  $R_{CSDA}$  electron ranges have been extracted from the ESTAR database<sup>6</sup>, as indicated in Figure 1.

PENELOPE v. 2008 main code databases provide a large list of different materials along with the corresponding radiation-matter interaction properties. As mentioned above, scaled DPK have been calculated in water-equivalent spherical phantoms which physical and geometrical properties have been introduced by means of the MATERIAL and PENGEOM packages, respectively.

## Results and discussion

After preliminary consistency tests, the dedicated Monte Carlo subroutine has been used for the calculation of in-water energy deposition of monoenergetic sources. A set of isotropic point sources emitting 10 keV, 50 keV, 100 keV, 500 keV, 1 MeV and 3 MeV electrons has been considered with the aim of covering the energy range of interests for typical beta-minus radionuclides used in nuclear medicine treatments. A typical result for energy deposition distribution is reported in Figure 2.

From such results for the energy deposition within concentric shells, it becomes straightforward to obtain the scaled DPK by means of Eq. 3 using shell radius as travelled path  $s$ .

As example of the capability of the developed calculation system to attain primary and scattering contributions separation, Figures 3 to 6 show the scaled DPK results obtained for a monoenergetic case along with three typical radionuclides used in nuclear medicine treatments.

In the case of radionuclides, the traveled path  $s$  has been normalized to the corresponding spectrum weighted CSDA range ( $\langle R_{CSDA} \rangle$ ). Similarly, the energy value  $E_0$  used for

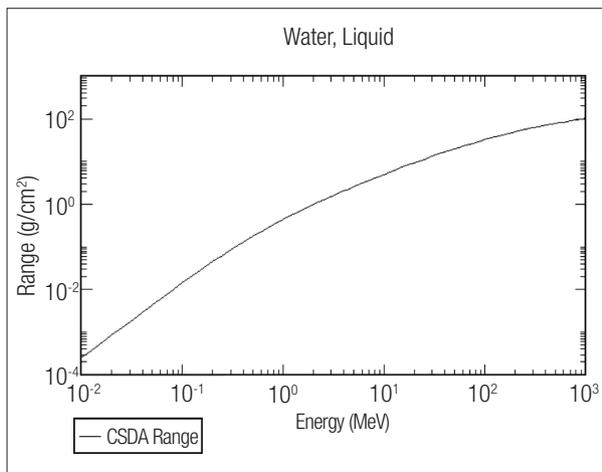


Figure 1. ESTAR  $R_{CSDA}$  for liquid water.

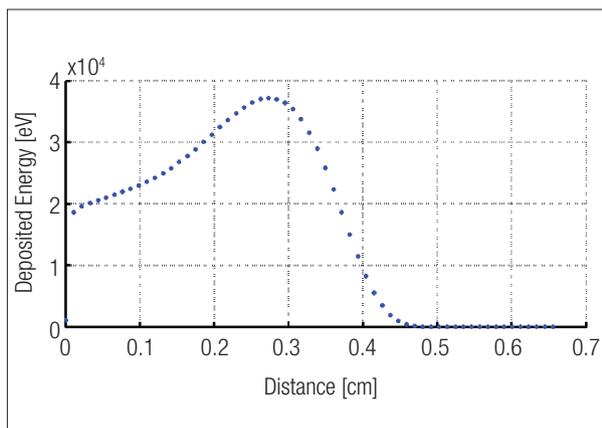


Figure 2. Energy deposition mean value for 1 MeV electron source as function of distance to the point source.

deposited energy normalization within shells has been calculated according to the spectrum weighted mean value.

As reported in Figures 4 to 6, the relative contribution from scattering radiation to total scaled DPK depends strongly on radionuclide emission properties.

According to the obtained results (Figures 3 to 6) it can be established that each investigated radionuclide presents different relative distribution between the primary and scattering contributions to the total scaled DPK.

However, it was found in all cases that there is a non uniform relative scattering contribution among distance to point source, therefore meaning that scattering to primary ratio needs to be calculated at any distance from point source.

The calculations performed with the dedicated subroutine used absorption energy at 1 keV as fixed threshold value, except for the 10 keV source for which an absorption value of 0.1 keV was considered. This criterion allowed to ensure that simulated showers have been appropriately transported until kinetic energy reduced to values, at least, hundred times lower than the initial one. The absorption energy represents the lower limit for the particle kinetic energy that has to be simulated. Once a particle reduces its kinetic energy to this threshold value, it is

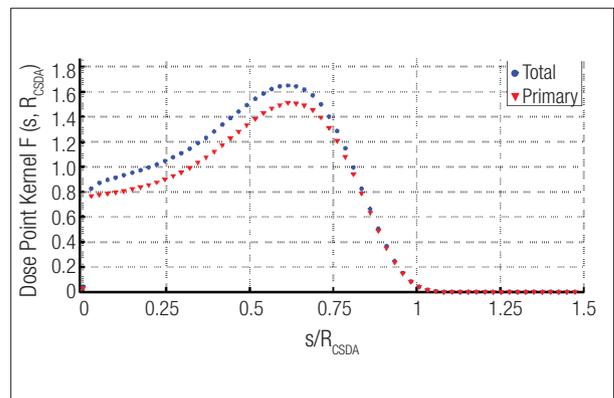


Figure 3. Separation of primary contribution (solid red triangles) from total (solid blue circles) scaled DPK for 1 MeV electron source.

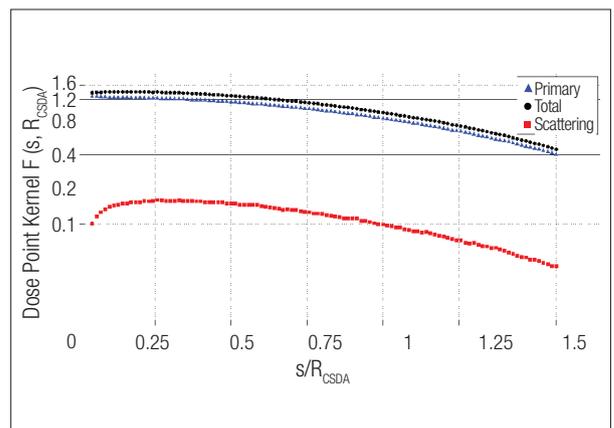
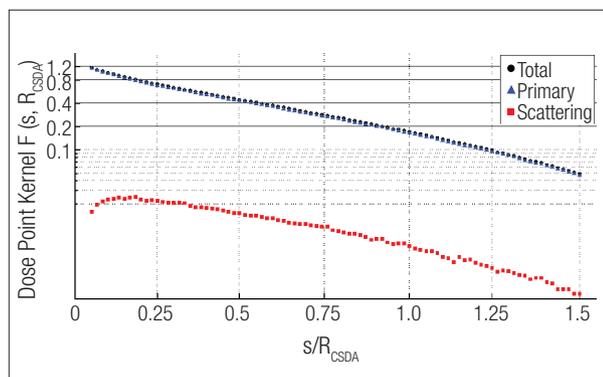
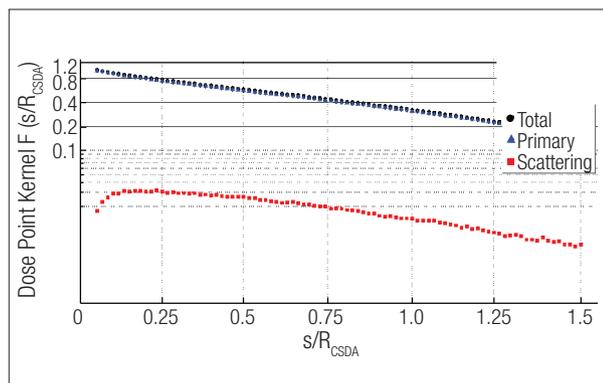


Figure 4. Separation of primary (solid blue triangles) and scattering (solid red squares) contributions from total (solid black circles) scaled DPK for  $^{90}\text{Y}$  source, using  $R_{CSDA} = 0.432$  cm in water.



**Figure 5.** Separation of primary (solid blue triangles) and scattering (solid red squares) contributions from total (solid black circles) scaled DPK for  $^{177}\text{Lu}$  source, using  $R_{\text{CSDA}} = 0.025$  cm in water.



**Figure 6.** Separation of primary (solid blue triangles) and scattering (solid red squares) contributions from total (solid black circles) scaled DPK for  $^{131}\text{I}$  source, using  $R_{\text{CSDA}} = 0.040$  cm in water.

“locally absorbed”, which means that the residual energy (less than the user defined absorption energy) is locally deposited and the particle tracking is considered to be finished.

Actually, disregarding the radionuclide type, greater relative scattering contributions have been found at short scaled distances, *i.e.* concentrated quite around the isotropically emitting point source. In addition, contrary to the case of monoenergetic sources for which maximum of relative scattering contribution correspond to deeper penetration distances, the obtained results show that, in the case of radionuclides, the maximum of relative contribution from scattering to total scaled DPK happened for scaled distances close to 0.2, which means 20% of the actual effective CSDA range ( $\langle R_{\text{CSDA}} \rangle$ ). This fact may arise from the combination of different energy channels each one having its own penetration capacity until particle thermalization. In addition, both monoenergetic sources and radionuclides have shown the same behavior regarding the decreasing tendency for the relative scattering contribution at large distances, as expected.

## Conclusion

A novel calculation system along with corresponding Monte Carlo subroutine has been developed. The first consistency

tests regarding monoenergetic electron sources have preliminary shown the viability of the proposed calculation method. Moreover, it has been satisfactory benchmarked when applied some radionuclides typically used in nuclear medicine treatment. At the moment, efforts are devoted for extending the proposed method to other radionuclides appropriate for nuclear medicine, like  $^{89}\text{Sr}$ ,  $^{153}\text{Sm}$ ,  $^{186}\text{Re}$  and  $^{188}\text{Re}$ . In base on the preliminary tests and the obtained results, the purposed method seems to be a suitable and promising tool for assessing primary and scattering contributions to total energy deposition for calculating scaled dose point kernels in nuclear medicine. Furthermore, the proposed method can be improved in order to distinguish even between the different components of the scattering contribution to total DPK, according to the corresponding interaction mechanism.

It has been found, as it is well-known, that primary and scattering energy fluences are significantly different at any location within the irradiated phantom, therefore it may be expected that the corresponding differences in linear energy transfer (LET) and ionization properties would affect the net energy deposition. In addition, due to intrinsic physical properties, suitable distinction between primary and scattering contributions may be particularly useful for clinical dosimetric purposes because this information may be used for improving radiobiological calculations, like tumor control probability (TCP) and normal tissue complication probability (NTCP).

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