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1 **Dose Point Kernels in liquid water:**

2 **an intra-comparison between GEANT4-DNA and a variety of Monte Carlo codes**

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19
20 **Abstract**

21 Modelling the radio-induced effects in biological medium requires accurate physics models to
22 describe in detail the main physical interactions induced by all the charged particles present in
23 the irradiated medium (secondary as well as primary ones). These interactions include
24 inelastic events like ionization and excitation processes as well as elastic scattering, the latter
25 being the most important process in the low-energy regime. To check the accuracy of the

26 theoretical models recently implemented into the Geant4 toolkit for modelling the electron
27 slowing-down in liquid water, the simulation of electron Dose Point Kernels remains the
28 preferential test. In this work, normalized radial profiles of deposited energy at a distance
29 from emissions point sources are then computed in liquid water by using the very low energy
30 “Geant4-DNA” physics processes available in the Geant4 toolkit. We here report an extensive
31 comparison with profiles obtained by a large selection of existing and well-documented
32 Monte-Carlo codes, namely, EGSnrc, PENELOPE, CPA100, FLUKA and MCNPX.

33

34 **Keywords:** Dose Point Kernel; Geant4-DNA; Monte Carlo codes; liquid water.

35

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46

47 **1. Introduction**

48 Energy deposition functions from point isotropic sources - commonly denoted dose point
49 kernel (DPK) functions - are of prime interest in many fields like dosimetry in particular for
50 medical applications. To better understand the radiobiological effects resulting from the use
51 of electron-emitting radiopharmaceuticals, it is necessary to have an appropriate knowledge of
52 the cellular distribution of the radiopharmaceutical and then to model the microscopic
53 distribution of energy deposited in irradiated matter [1]. Absorbed doses to targeted cancer
54 cells play an important role in evaluating the relative merits of different radionuclides and
55 pharmaceuticals. In this context, information on the bio-distribution at the tissue, cellular and
56 sub-cellular levels can be obtained by autoradiography [2], micro-autoradiography [3], or
57 alternative techniques such as secondary ion mass spectrometry [4]. Converting these data to
58 absorbed dose distribution requires the use of analytic methods based on point-dose kernels or
59 methods based on radiation transport calculations [5-7]. Indeed, Monte Carlo code event-by-
60 event simulations can be particularly suitable [7-11]. The latter consist in describing, step-by-
61 step, interaction after interaction, the history of each ionizing particle created during the
62 irradiation of the biological matter. In this kind of numerical code, each projectile-target
63 interaction is described either thanks to theoretical (differential as well as total) cross sections
64 or by semi-empirical ones giving access to a more or less complete description of the
65 kinematics before and after the collision.

66 In fact, there are in the literature a large number of Monte Carlo electron track-structure
67 codes in water, which have been developed independently to investigate the microscopic
68 features of ionizing radiation, the ensuing chemical pathways and the molecular nature of the
69 damages in bio-molecular targets (see [11] and references therein). The aim of the present
70 study is to compare dose point kernels - for particular electron energies - calculated by using
71 different Monte Carlo codes, namely, EGSnrc [12], PENELOPE [13], CPA100 [14], FLUKA

72 [15], MCNPX [16] and GEANT4-DNA [17]. To do that, the energy deposited by the emitted
73 electrons as well as all the secondary particles produced along the primary trajectories are
74 scored in spherical shells placed around an isotropic source for distances ranging from 0 to
75 1.2 times the continuous slowing-down approximation range hereafter denoted R_{CSDA} and
76 provided by the different codes here studied.

77

78 **2. Methods**

79 The Monte Carlo numerical simulations used in the present study are well-documented and
80 nowadays extensively used by many groups. Only a brief description is then hereafter
81 reported and for more details we refer the interested reader to the corresponding literature
82 whose examples are cited as references.

83 *2.1 The GEANT4-DNA code*

84 The Geant4-DNA code is fully included in the general purpose Geant4 Monte Carlo
85 simulation toolkit. It simulates track structures of electrons, hydrogen and helium atoms of
86 different charge states (H^0 , H^+) and (He^0 , He^+ , He^{2+}) respectively, as well as C^{6+} , N^{7+} , O^{8+} and
87 Fe^{26+} ions, in liquid water. The physical processes include ionization (for all particles),
88 electronic excitation (for electrons, protons, hydrogen atoms and α -particles including their
89 different charge states), charge exchange (for hydrogen and helium atoms with the above-
90 mentioned charge states), and, for electrons, elastic scattering, vibrational excitation and
91 dissociative attachment. Electron interactions cover the 7.4eV - 1MeV energy range, whereas
92 proton and hydrogen interactions are simulated from 100eV to 100MeV while helium ions of
93 different charged states are followed from 1keV up to 400MeV. These processes are further
94 described in [17].

95 *2.2 The EGSnrc code*

96 EGSnrc is a general-purpose package for the Monte Carlo simulation of the photons and the
97 electrons transport from a few keV up to 100GeV. EGSnrc uses a condensed history approach
98 based on the formalism developed by Kawrakow and Bielajew to sample angular distributions
99 from the any-angle form of the screened Rutherford cross section [18]. The Möller inelastic
100 cross-sections are used for the generation of secondary electrons. For this study, the
101 simulations were based on the user-code EDKnrc developed by Mainegra *et al.* [19]. We
102 applied the PRESTA II electron-step algorithm and the EXACT boundary crossing algorithm
103 to switch to single scattering when a particle comes closer to a boundary. The “skin depth”
104 parameter was set to 3: it represents the number of elastic mean free paths to the next
105 boundary at which the simulation switches into single scattering mode. We set the cut-off
106 parameter ECUT to 1 keV in order to track primaries and secondaries until they leave the
107 geometry or their energy falls below 1 keV. We produced a PEGS4 data set describing cross
108 sections and stopping powers adapted for this low cut-off value.

109 *2.3 The PENELOPE code*

110 PENELOPE (2006 version) is a general-purpose Monte Carlo code for the coupled simulation
111 of electron and photon transport. The cross sections database used in PENELOPE covers a
112 wide range of elements ($Z = 1-99$) and various materials useful for medical applications in the
113 energy range of 50 eV - 1 GeV. This code has the flexibility to generate electron and positron
114 histories on the basis of a mixed procedure, which combines detailed simulation of hard
115 events with the continuous slowing down approximation for soft interactions. The level of
116 detail of electron transport processes is controlled in PENELOPE by specifying values for
117 several parameters, C_1 , C_2 , W_{CC} and W_{CR} . The C_1 and C_2 parameters are associated to the
118 condensation of electron and positron elastic scattering processes. W_{CC} and W_{CR} , respectively,
119 represent the cut-off energy losses for hard inelastic collisions and for hard Bremsstrahlung
120 emission. A detailed description of the algorithms used in PENELOPE can be found in its

121 manual [20]. These simulations were done with detailed event-by-event transport setting
122 $C_1 = C_2 = 0$, $W_{CC} = W_{CR} = 50$ eV and using 50 eV as the lower absorption energy allowed in
123 this code.

124 *2.4 The CPA100 code*

125 CPA100 is an event by event Monte Carlo track structure code, developed in Toulouse
126 (France), for understanding fundamental aspects of radiation track interaction [14]. It
127 simulates complete electron/photon transport in liquid water for energy range from 10 to
128 200 keV. It generates all the electronic and photonic cascades occurring after a particle
129 passage in the volume of interest (Auger electron, X-Rays, atomic reorganization). It is also
130 able to describe the various stages of the particle transport not only the early physical stage,
131 but also the physico-chemical and the chemical ones, during the very early passage of
132 particles in matter say up to one microsecond. Primary physical and chemical damages not
133 only in liquid water but also in complex DNA targets and its higher order structures can be
134 calculated to estimate the radio-induced damage to the DNA molecular scale (DSB, SSB,
135 base lesion).

136 *2.5 The FLUKA code*

137 FLUKA is a multi-purpose Monte Carlo particle transport code that considers all particle
138 interactions including electromagnetic interactions, nuclear interactions of the primary or
139 incident particles and the generated secondary particles, energy loss fluctuations and Coulomb
140 scattering [15]. The version 2011.2.15 with the default configuration 'PRECISION' was used,
141 with an energy cut-off lowered at 1 keV for electrons and 0.1 keV for photons. To reach a
142 good accuracy, the single scattering model through the 'MULSOPT' option was activated,
143 because the Moliere multiple scattering model could be unreliable with thin shells, disturbing
144 the propagation of electrons between the boundaries [21].

145 *2.6. The MCNPX code*

146 MCNPX is a general-purpose Monte Carlo code for modelling the interaction of radiation
147 with matter [16]. MCNPX stands for MCNP eXtended and transports electrons, photons,
148 neutrons and several particle types, like nearly all energies. It utilizes the latest nuclear cross
149 section libraries and covers various materials useful for medical applications. The tallies have
150 extensive statistical analysis and the convergence is enabled by a wide variety of variance
151 reduction methods. For this work, the version 2.7.0 was used with the F8* energy deposition
152 tally in coupled electron-photon mode. The photon and electron cut-off energies were set
153 above 1 keV. A specific consideration was focused on electron transport conditions, through
154 the ITS option and the ESTEP parameter, due to the very narrow shells. The ITS energy
155 indexing algorithm was used to have a better definition of the energy group and their
156 boundaries [22] and the ESTEP parameter was increased in order to divide the major electron
157 energy step into smaller sub-steps [23]: ESTEP = 10 for 100 keV and ESTEP = 100 for 10, 30
158 and 50 keV.

159

160 **3. Results and discussion**

161 To obtain the dose point kernel (DPK) around an isotropic point source, the geometry
162 here used consists in a spherical water phantom divided into 120 spherical shells of thickness
163 $R_{CSDA}/100$, where R_{CSDA} stands for the continuous-slowing-down-approximation range whose
164 values calculated by the different codes here studied are reported in Table 1. Note that for the
165 EGSnrc, the CPA100, the FLUKA and the MCNPX codes, the corresponding values are taken
166 from the NIST web database ESTAR [24], what generates stopping powers and ranges for
167 electrons which are the same as those tabulated in ICRU Report 37 [25]. Besides, let us
168 remind that the present GEANT4-DNA version transports electrons down to an energy
169 threshold of 7.4 eV contrary to the other codes studied which use higher energy cut-off, what
170 undoubtedly affects the R_{CSDA} values.

171 Finally, the GEANT4-DNA DPK distributions have been compared to those obtained
172 with the other Monte Carlo codes by using Kolmogorov-Smirnov statistical tests. Thus, we
173 found that the GEANT4-DNA simulations are statistically compatible with EGSnrc and
174 PENELOPE simulations (p -value > 0.05) with a maximum distance (D) between distribution
175 functions less than 0.2. On the contrary, much smaller p -values (< 0.05) and larger D
176 distances were obtained when comparing GEANT4-DNA simulations with the MCNPX and
177 CPA100 simulations.

178 The DPK distributions also obtained by the different numerical codes are reported in
179 Figure 1 for four particular electron energies, namely, 10 keV, 30 keV, 50 keV and 100 keV.
180 These quantities are defined as the fraction of the emitted energy absorbed (per unit mass) at a
181 certain distance from the point source and are usually reported by means of scaled
182 distributions defined as $F(r/R_{CSDA}) = \frac{\delta E(r)/E_0}{\delta r/R_{CSDA}}$ where r is the distance from the point source,
183 $\delta E(r)$ stands for the energy absorbed in the spherical shell sited at a distance r from the point
184 r/R_{CSDA} source, E_0 being the initial kinetic energy of the electron and δr the shell thickness
185 (here $R_{CSDA}/100$). The obtained distributions will be hereafter reported as a function of r/R_{CSDA}
186 and refer to scoring of the deposited energy at the mid-radius of the shell.

187 In Figure 1, we observe that the shape of the dose point kernels generated by the
188 different codes is very similar. However, we note that the CPA100 code exhibits a peak closer
189 to the source in comparison to the other codes ($r/R_{CSDA} \cong 0.53$ vs 0.58), the amplitudes being
190 all of the same order of magnitude - from 1.45 to 1.55 - except for the MCNPX which largely
191 overestimates the other results. When the incident electron energy increases, these
192 observations are confirmed with in particular an improvement of the agreement between the
193 CPA100 and the other simulations. Thus, from Fig.1b) to Fig.1d) all the curves tend to
194 converge except again the MCNPX simulation which provides higher DPKs (of about 20%).

195 Besides, for the four energetic cases here reported, the GEANT4-DNA DPK
196 distributions have been compared to those obtained with the other Monte Carlo codes by
197 using Kolmogorov-Smirnov statistical tests. Thus, we found that the GEANT4-DNA
198 simulations are statistically compatible with EGSnrc, PENELOPE and FLUKA simulations
199 (p -value > 0.05) with a maximum distance (D) between distribution functions less than 0.3.
200 On the contrary, much smaller p -values (< 0.05) and larger D distances were obtained when
201 comparing GEANT4-DNA simulations with the MCNPX (for the four incident energy
202 values) and CPA100 (for 30 keV and 50 keV) simulations.

203 204 **4. Conclusions**

205 Normalized radial profiles of deposited energy - commonly referred to as dose point kernels -
206 have been here reported by using the very low energy “Geant4-DNA” physics processes
207 available in the Geant4 toolkit. In comparison with profiles obtained by a large selection of
208 existing and well-documented Monte-Carlo codes, namely, EGSnrc, PENELOPE, CPA100,
209 FLUKA and MCNPX, we have here emphasized evident discrepancies undoubtedly related to
210 the physics models implemented into the different codes. In this context, the Geant4-DNA
211 code has been shown to provide accurate dose point kernels for incident electron energies
212 ranging from 10 keV to 100 keV.

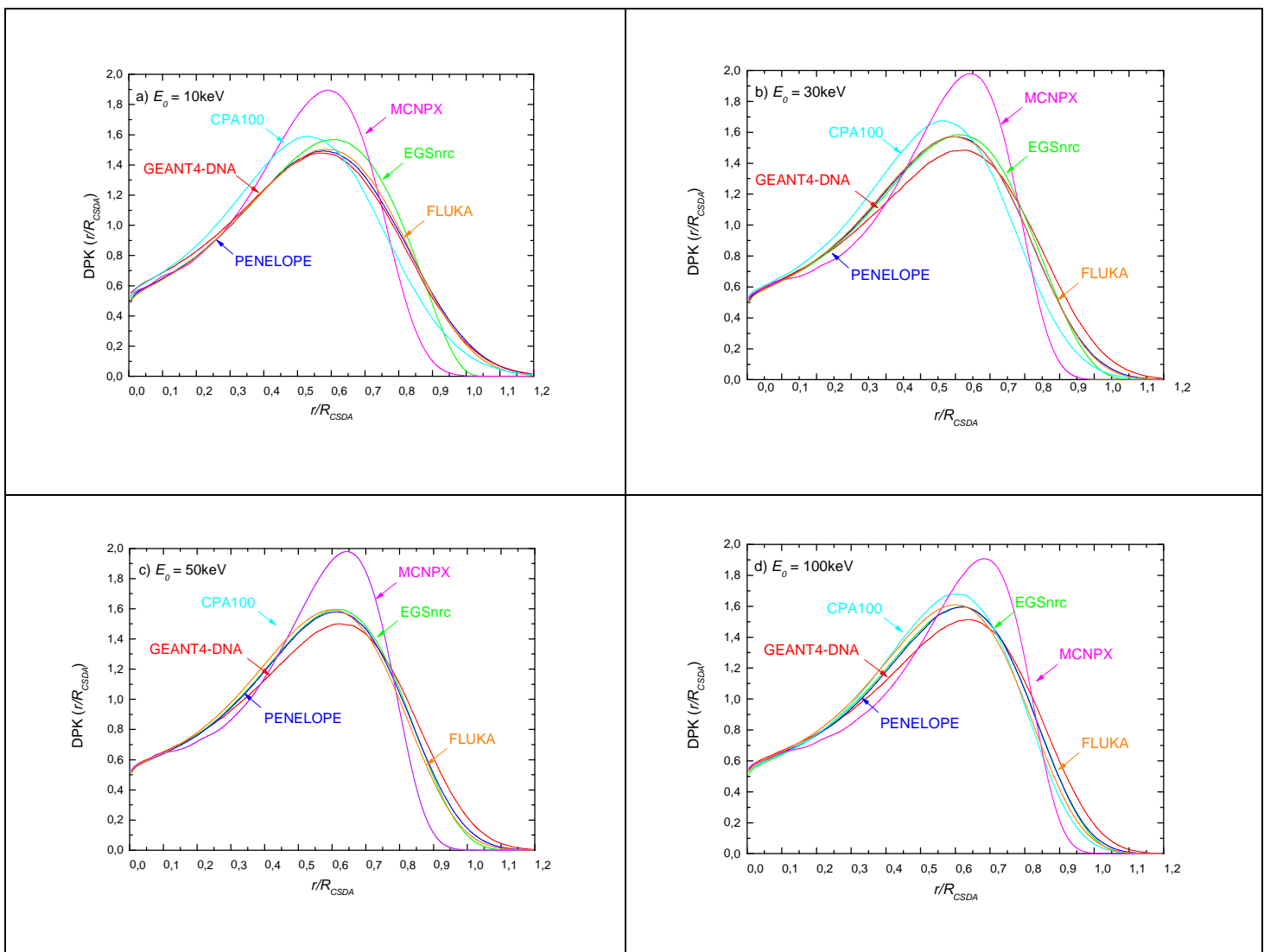
213 214 **Acknowledgements**

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219 Recherche Scientifique.

220 **Figure 1:**

221 (Color online) Comparison between the scaled dose point kernel distributions obtained by the
222 different numerical track-structure codes studied in the present work: GEANT4-DNA (red),
223 EGSnrc (green), PENELOPE (blue), CPA100 (cyan), MCNPX (magenta) and FLUKA
224 (orange). Panel a) $E_0 = 10$ keV. Panel b) $E_0 = 30$ keV. Panel c) $E_0 = 50$ keV.
225 Panel d) $E_0 = 100$ keV.

226



227

228 **Table 1:**

229 Comparison between the continuous-slowing-down-approximation range R_{CSDA} (μm) obtained
230 by the different numerical track-structure codes studied in the present work.

E_0	R_{CSDA} (GEANT4-DNA)	R_{CSDA} (PENELOPE)	R_{CSDA}^* (EGSnrc, CPA100, KLUKA, MCNPX)
10 keV	2.76	2.52	2.52
30 keV	18.16	17.57	17.56
50 keV	44.07	43.21	43.20
100 keV	144.12	143.06	143.10

231 **Note that the EGSnrc, CPA100, FLUKA and MCNPX values have been taken from the NIST*
232 *web database ESTAR [24] contrary to the other data here reported.*

233

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