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ELECTRON ABSORBED DOSE COMPARISON BETWEEN MCNP5 AND PENELOPE MONTE CARLO CODE FOR MICRODOSIMETRY

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ABSTRACT

The objective of the present work was to compare electron absorbed dose results between two widespread used codes in international scientific community: MCNP5 and Penelope-2003. Individual water spheres with masses between 10^{-9} g up to 10^{-3} g immersed in an infinite water medium (density of 1g/cm^3) and monoenergetic electron sources with energy from 0.002 MeV to 0.1 MeV have been considered. The absorbed dose in the spheres was evaluated by both codes and the relative differences have been quantified. The results shown that Penelope gives, in general, higher results that, in some cases saturate or reach a maximum point and then rapidly drops. Particularly, for the 40 keV electron source we have done additional tests in three different scenarios: a) more points in the region of lower masses to a better definition of the curve behavior. b) MCNP used 200 substeps and Penelope was set to a full detail history methodology and c) almost same parameters of case B but with the density of exterior medium increased to 10 g/cm^3. The three cases show the influence of the backscattering that contribute with an important fraction of absorbed dose, finally we can infer a range of reliability to use the codes in this kind of simulations: both codes can calculate close results for up to 10^{-4} g.Even though MCNP5 uses the condensed history method, if simulation parameters are chosen carefully it can reproduce results very close to those obtained using detailed history mode. In some cases, the use of higher number of electron substeps causes significant differences in the result.

1. INTRODUCTION

In 1963, Berger developed the condensed histories method for charged particles transport particularly for electrons[1]. This opened the possibility of implementation of computer algorithms that allowed the simulation of interaction of charged particles with matter in a reasonably efficient time. As a result of this new approach the ETRAN code[2,3] was developed. This code has been widely used in dosimetric studies and later incorporated by the MCNP Monte Carlo code in its latest versions[4]. The use of history condensed methodology is currently a common resource for all major Monte Carlo codes available as Penelope[5], Geant[6], EGSnrc[7] and the aforementioned MCNP.

The condensed history method allied with the huge advance in computational power and reliability led to a fast and wide spring of MC codes enabling simulation of more complex problems, including those of medical physics relevance. As the result computational dosimetry area received great attention with an increase demand of work[8].

More recently, a new class of problems in absorbed dose calculation is being increasingly exploited by the Monte Carlo codes, the microdosimetry, where the geometry size of the simulation is no longer the order of organs' size or tissue as stipulated by the Medical Internal Radiation Dose (MIRD), but to cells or even the DNA itself[9,10,11]. This new approach takes the codes to their simulation capability limits and therefore further studies remains to be done to explore the actual limitations of such codes in this new environment.

In this context the present study aims to compare two major Monte Carlo codes for the radiation transport currently available and with growing interest in the area of dosimetry: Penelope-2003 and MCNP version 5. Penelope has received some prominence in microdosimetry utilization while MCNP is widely used for several applications including reactor and medical physics. In the present work, both codes were used to calculate the absorbed dose in spheres of water with masses from 10^{-9} to 10^{-3} g immersed in an infinite volume of water. Electron sources with energies from 2 to 100 KeV, homogeneously distributed in the sphere were considered. Also, to simulate the variation of tumor sizes in healthy tissues, we designed a cluster of spheres equivalent to a 9x9x9 size matrix of water spheres. For these simulations, the electron source was inserted only in the central sphere and the dose was evaluated in all 729 spheres. MCNP5 used the condensed history algorithm while PENELOPE code has the ability to simulate condensed and individual electron stories so that the results were compared as well the time for using the two methodologies.

2. METHODS

2.1. The Penelope-2003 code

The Penelope code is a mixed simulation algorithm[6] capable of simulate couple electron-positron particles from ~0.1 keV up to ~1 GeV. This means that it can separate the methodology used following a predetermined threshold of energy loss defined by the user, above this threshold interactions of electrons are called "hard" and treated with the rigor of individual simulation. The "soft" interactions are treated with condensed histories methodology. For photons the histories are simulated with detailed histories method.

The code is written in Fortran 77 language in a modular pattern, which means that it has a "kernel" or the software itself, responsible for all the physics of the particle transport, a material module responsible for the elements, densities involved and their respective stopping power and cross sections data and a module with all the geometric surfaces and composition of each part of the bulks (modules or bodies). In this work, the PenEasy a general-purpose main program for Penelope that significantly simplified the assembly and the set of parameters in simple problems[12] has been used to make the input.

The great versatility of this code, providing the mixed simulation methodology and the capability of simulate and follow the history of eletrons-photons with low energies has shown to be an interesting combination for microdosimetry area.

2.2. The MCNP version 5 code

MCNP code was created in the fifties to simulate neutrons and photons in reactors by the Los Alamos National Laboratory. Afterwards, the Integrated Tiger Series (ITS) indexing energy algorithm was incorporated after the MCNP4A using the ITS version 1.0, then MCNP

become a more complete code including electrons in its row of particles. Today MCNP uses the ITS version 3.0. This union allowed the code to be used in dosimetry studies.

This code has a powerful geometric capabilities, a relative easy interface and can simulate particles with energy from 10^{-11} MeV to 20 MeV for neutrons (and up to 150 MeV for some isotopes), from 1 keV up to 100 GeV for photons and from 1 keV up to 1 GeV for electrons. However, MCNP can only simulate electrons with the condensed history mode.

2.3. The models

Absorbed dose calculation has been done in water spheres with density of 1 g/cm^3 immerse in an infinite medium of water. The electron sources were located uniformly in the sphere. The initial particles energies considered are 0.002, 0.003, 0.004, 0.006, 0.008, 0.01, 0.02, 0.03, 0.04, 0.06, 0.08 and 0.1 MeV. The mass of spheres were 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8} and 10^{-9}g.

2.4. Simulation

All the simulations for the single spheres were executed with 10^6 histories reaching relative error below 0.5% (which can be considered negligible for this work) without any variance reduction technique. The electrons were followed until 0.1 keV (actually depend on the particle as will see later for Penelope) or 1 keV (for MCNP). Below these cut off energies the codes consider a local energy deposition and stop that history going to the next one.

MCNP used respectively the “el1” and “mcplib04” electron and photon libraries and two options for the energy indexing algorithm: the default and the ITS indexing mode. Some works[13,14] have shown that a systematic error in results are introduced when the default option is used, so that, in the present work all calculation were done in ITS mode. The energy deposition, *F8 tally was used to evaluate the absorbed dose as a product of pulse height tally (F8) by the total energy deposited by a history in the bulk of detection. For the present analysis and specifically for 0.04 MeV, 10 substeps instead of 3 which is default was used. This choice was made to have a little improvement on the results for the electrons as demonstrated by D.R. Schaart *et al*[14].

Penelope was used with the PenEasy extension and configured to use the cut off angle that distinguishes soft and hard collisions parameter (C1 and C2) as 0.1.The cut off energies for Bremsstrahlung events (Wcr) and the production of hard collisions (Wcc) were respectively 100 and 1000 eV. The maximum step size (Dsmax) was taken as 10^{30} and the cut off energies for stop the history (Eabs) were 100 eV for electrons and positrons and 10 eV for photons. In later analysis for a full detailed simulation, the parameters used are:C1=C2=Wcc=Wcr=0. The best choice for each parameters are discussed either by J. Sempau and P. Andreo[15] or in Penelope manual.

3. RESULTS AND DISCUSSION

First, the Penelope run with parameters C1=C2=0.1 and Wcc=10xWcr=10^3, Dsmax=10^{30}, so that in these cases the code used condensed histories. MCNP used its default substep number

(3) and for 0.04 MeV or higher it was used 10 substeps to partially compensate the statistical loss of secondary particles[16].

After all simulations completed the absorbed dose in the spheres were compared choosing the MCNP values as reference values. Figure 1 shows the results.

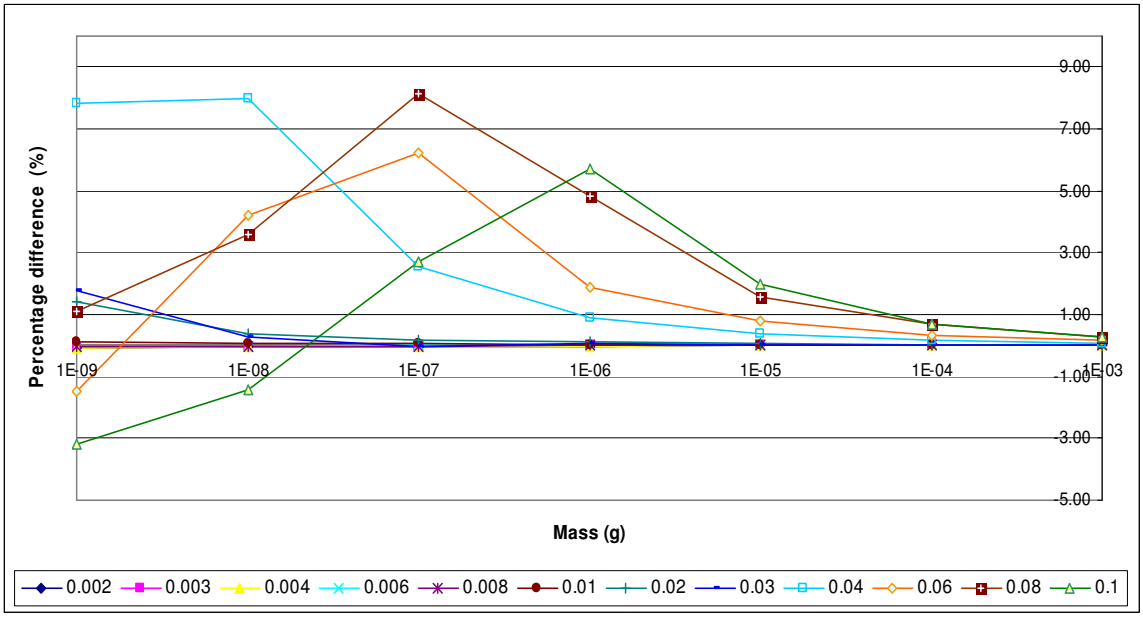

Figure 1. Percentage difference between Penelope and MCNP. Reference: MCNP.

One can note that Penelope tends to give higher values than MCNP except in very low masses (for this spheres dimension range). In general the curves behavior are always crescent until some threshold, reaching a level or an inflection point then starts to decrease giving even negative values for smaller spheres for highest energies (0.08 and 0.1 MeV). The biggest difference observed here was 8.16% for the 10^{-7} g sphere and source energy of 0.08 MeV curve.

For a deeper analysis of the discrepancies found for the energy of 0.04 MeV another series of experiments were made in a attempt to explain that behavior. To accomplish it three cases were simulated, namely:

- Scenario A: Exactly the same parameter, but with additional points, especially in lower masses;
- Scenario B: The simulation parameters of Penelope code were C1=C2=Wcc=Wcr=0 (detailed histories mode) and MCNP simulation using 200 substeps;
- Scenario C: Almost same parameters of case B but now the density of exterior medium increased to 10 g/cm^3.

Figure 2 show the curves of each case, the first one show the same behavior of 0.04 MeV curve in Figure 1 as expected only with more points ($7x10^{-10}$, $3x10^{-10}$, 10^{-10}, $7x10^{-11}$, $3x10^{-11}$ and 10^{-11}). The second case seemed that has the same shape but with lower amplitude than case A, the data between the codes are more aggregated, resulting lower relative errors. At

last, case C curve clearly shows a “level” or a saturation range between 10^{-9} and $5x10^{-10}$ g in a different range than that observed in case A .

Comparison between the absorbed dose difference calculated with Penelope using mixed and full detailed history methodology (reference: mixed data) and the difference between standard (or 10) and 200 substeps using MCNP (normalized by standard substeps data) can be seen in Figure 3. The curves show that for Penelope results obtained with mixed history method or detailed method are neglibible (<0.5%), however for MCNP the results shown relative error variation between 10^{-6} and 10^{-10} g of up to +3.63% for different number of substeps (at least for this set of energy and masses). probably because the number of interactions neglected by any condensed methodology was partially offset by more substeps, beyond 10^{-10} g the differences are small again but just because both results reflects the massive lost of particles escaping so the results converge similarly to zero.

The small differences observed in the curve (a) of Figure 3 indicated that with appropriate parameters the condensed history method gives similar results than those obtained with detailed mode in PENELOPE> In second place curve (b) in Figure 3 show again that beyond a certain sphere sizes for each initial energy the particle number that interacts with the sphere is so small giving a poor statistic and both codes show a fast drop to negligible values in absorbed dose requiring at this point either increase the history number or the use of variance reduction techniques or if possible both resources.

At this point we can conclude that the higher absorbed dose obtained by Penelope observed both in Figure 2 and 3 is not due to the mixed/detailed algorithm over the condensed method present in MCNP, but probably the cause of these differences resides in the transport algorithm employed by the two codes reflecting a different backscattering contribution in total absorbed dose, obviously minor to MCNP. The higher density in the external medium results in a different mass range reinforcing the backscattering contribution to the dose.

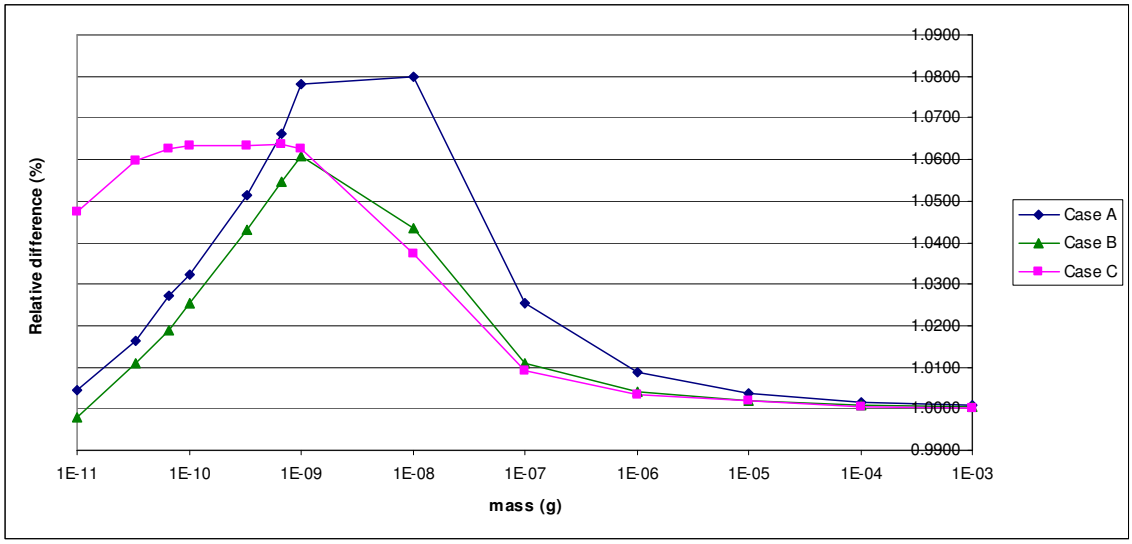

Figure 2. Three different cases or set of parameters of both codes, all values were related by MCNP data.

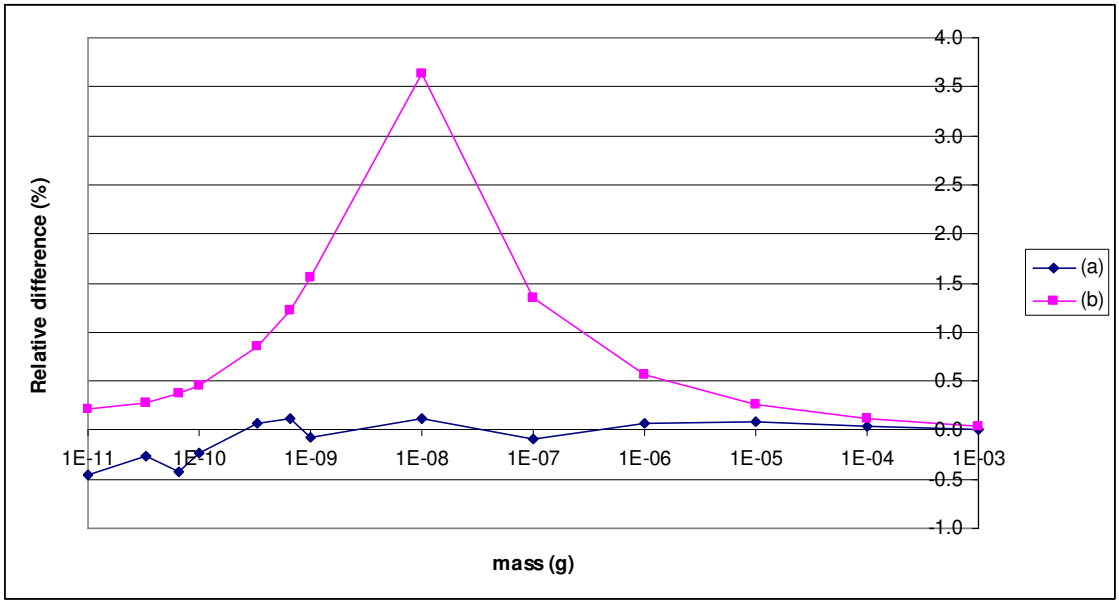

Figure 3. (a) Relative differences using Condensed and Detailed modes in Penelope to a 0.04 MeV set related by condensed data set. (b) Relative errors using 200 or 3-10 substeps, related by the standard data.

4. CONCLUSIONS

The use of stochastic approach to solve the transport equation to electrons using a condensed history method as suggested in the 60's by Berger allied to a huge development in the computational power led to a fast spread of codes as MCNP, EGS, Geant and Penelope in several areas from nuclear reactor core designs until medical physics as in dosimetric studies. This work has the purpose of make a comparison between two major codes widely used by the scientific community, MCNP version 5 and Penelope 2003 in a still few studied field, the microdosimetry. In general the MC codes are applied in a completely different range both in space as in energy, consequently the literature has almost none benchmarks or even works in this area, this increased interest is due the necessity of even more accuracy in absorbed dose distribution to develop future protocols or define more realistic phantoms.

These results showed a clear tendency: Penelope in almost all cases gave higher values than the MCNP. In Figure 1 we see a pattern for all those curves, in low masses both codes give close results but for the same energy with the initial energy increased gradually the results diverge (reaching even ~8.16 % with MCNP as reference) probably because the detailed history methodology do not underestimate the secondary particles created that eventually can deposit energy contributing to absorbed dose, this information is partially lost with a condensed history methodology as used by MCNP.

Another characteristic that we could note is that relatives differences reach a saturation level or a maximum point and then starts to a fast drop, probably because after this range (directly related with the mass of the sphere and energy of the source) almost all particles escape both secondary particles or the ones from the backscattering can not deposit any energy due the tiny bulk so the two codes give values that likewise go to null.

Some simulation parameters was change to see their impact in the results as the substep change in MCNP and threshold energy and scattering angle that separate "hard" of "soft" interactions in Penelope, in Figure 3 we can see that for the chosen parameter for Penelope the results differ very low (<0.5 %) but the substeps change can induce a sensitive difference in absorbed dose (maximum of +3.63 % in reference of standard substeps) this result was expected because the decrease of interactions neglected and consequently the secondary particles created (that in this scale is specially relevant) is partially compensated.

Finally is important note that these experiments do not have an experimental set to compare obviously because the dimensions of the problems in microdosimetry makes impossible some practical experiment that we could use to support therefore the numerical absorbed dose values calculated by MCNP and Penelope, so all analyses are just relative. All the simulations did not take more than 3 hours each for the cases with most costly parameters for processing as many substeps or full detailed methodology in a usual PC (Pentium D 3.00 GHz).

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