Investigation of Interactions Between Low Energy Positrons and DNA Using the Monte-Carlo Method

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ABSTRACT

Positron Emission Tomography (PET) is the imaging system used to diagnose an illness. Positrons from a radioactive nucleus are injected into the patient. There are few existing papers on the energy loses of positrons especially with low energy in the biological target. So, in this study, the goal was to investigate how low kinetic energy positrons (20eV-10keV) interact with DNA by using the Monte-Carlo simulation. In the simulation, screened Rutherford scattering Formula where Wentzel screening parameter was used for elastic collisions, algorithm proposed for the electron-matter interactions of re-edited version of positron interaction was used for inelastic collisions. Because positron-matter interaction involves randomness, the simulation was done using the Monte Carlo Method. In this simulation the screened Rutherford scattering formula using Wentzel screening parameters for elastic collisions and the electron-matter interaction model suggested by Liljequist for inelastic collisions were rearranged in order to determine positron interaction. The stopping powers of adenine, guanine, thymine, cytosine compounds and DNA were determined and compared with that of other related results. The results were found to be considerably higher than reported in some other papers.

Key Words: Positron, Monte-Carlo Method, Stopping power, DNA

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1. Introduction

Knowing how ionizing radiation, which is becoming increasingly used today, affects biological targets is vitally important for the field of healthcare. Systems where radiation is used in a controlled fashion are being developed for diagnosis and treatment purposes in the field of medicine. One such system is the Positron Emission Tomography (PET) imaging system. Developed as a cranial imaging system, PET together with CT has become particularly important in recent years in that it enables neuroscientists to monitor brain activity visually. Therefore, examining the basics and the details of how positrons affect biological targets is very important in terms of achieving the desired goal of the study and in increasing quality. When the stopping power of the biological target is known the best choice of shielding to be used to protect from radiation can be made, and it will be known how soon the radiation becomes harmless, meaning when its effects will end.

When a positron encounters an electron of almost equal energy while moving it can create an unstable positronium atom and it quickly gets destroyed producing gamma rays in the process.

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In other words, just as with all ionized radiation forms the positron's interaction with the target is a multi-part problem having complex analytic solutions. Such a problem should be studied using both classical and quantum mechanical methods. A Hans Bethe and Felix Bloch (Bethe, 1930; Bloch,1933) created an analytic expression based on the Born (1948) approach. This expression is still used in many studies. A semi-classic solution, it was proposed by Gryzinski in 1964 and has been known to be used by some researchers. Inokuti proposed a model based on the Generalize Oscillator Strengths (GOS) definition in 1971. This has found wide acceptance. This problem has been worked on in recent years with computers using the Monte Carlo Method because of the stochastic nature of the interaction between radiation and matter, and results are being obtained that are close to experimental results. PENELOPE (*PENetration and Energy Loss of Positrons and Electrons*) is one such program. When studies of stopping power are examined it is understood that the results do not match particularly in the low energy region. Most of the analytic solutions are unable to determine reasonable stopping power values in the low energy range (<10keV) (Berger and Seltzer, 1983; ICRU Report, 37, 1984).

In this study the Monte Carlo method was used to determine the elastic and inelastic interactions of low- and medium-energy positrons interacting with a biological medium throughout the period until they stop, to determine the frequency of these interactions and to calculate the medium's stopping power for positrons. While conducting the simulation for elastic collisions the screened Rutherford Scattering Formula and the screening parameters derived by Wentzel were used (Tökesi and Mukoyama, 1994). For the simulation of inelastic collisions the model suggested by Inokuti based on Generalized Oscilator Strength (1971) and simplified by Lilijequist (1983, 1984) was used.

The simulation was applied to water first for test purposes. The stopping power of such DNA components as the composites adenine, guanine, thymine and cytosine were calculated and the results for a biological cell with DNA were obtained.

2. Theoretical concepts for scattering events

Scattering events are studied using mathematical expressions called differential cross sections that denote the force, energy and directional changes between the particles that are sent to the target and the particles that are scattered off the target.

While the particles that undergo interaction as a result of elastic collision do not undergo any change to their internal structure, changes are observed in the direction of movement for particles having low mass. The Screening Rutherford Scattering Formula (differential cross section) for elastic interaction is given as follows:

$$\frac{d\sigma}{d\Omega} = \frac{Z^2 e^4}{4E^2(1-cos\theta+2\eta)^2} \qquad (2.1)$$

(Tökesi and Mukoyama, 1994). Where, Z, θ, e and E are atomic number, scattering angle, positron charge and kinetic energy of positron respectively. The atomic screening parameter reported by Wentzel (1926) is given,

$$\eta = \frac{3.4\, Z^{2/3}}{E} \qquad (2.2)$$

(Tökesi and Mukoyama, 1994). The total elastic scattering cross section as a function of positron energies by integrating over the entire scattering angle, σ_e is given as (Tökesi and Mukoyama, 1994);

$$\sigma_e = \frac{\pi Z^2 e^4}{4E^2\eta(\eta+1)} \qquad (2.3)$$

The mean free path for elastic scattering, λ_e is given,

$$\lambda_e = \frac{A}{N_a \rho \sigma_e} \quad (cm) \qquad (2.4)$$

Where A, is the atomic number of target material; N_a is Avagadro number, ρ is density of target material; σ_e is elastic scattering cross section.

In inelastic interactions the target atom is either excited to a suitable higher level than the ground level or it is ionized depending on the energy that the arriving particle imparts to the target atom. At the same time the arriving particle loses energy and move off in a different direction from the direction it came in. For positron-target interaction the target model is accepted as being homogeneous, amorphous and comprised of randomly distributed atoms or molecules. It is accepted that the atoms or molecules are at their ground states. If the atom

is going to be excited to a higher level this will be the highest permitted level because it is accepted right at the start that all the other lower levels are going to be occupied and that these levels are impassable.

If the target is an element then in the modelling of the target it is accepted that the electrons exist in shell upon shell as is known from quantum physics. The main shell and the sub-shells are called 1s, 2s 2p etc. In composites the total of the outermost shells of the materials that make up the composite are knows as the outer shell while the shell that is made up of the rest is known as the inner shell. Usually, the final shell is known as the valence shell (Lee *et al.,* 1990; Akar, 2005). The W_i resonance energy possessed by every shell is a characteristic for the target that is being used and it is important in inelastic interactions. W_i resonance energy is the amount of energy required for the electron in any shell to cross to the highest permitted level by being given energy in some way. In targets having a composite structure the grouping is generally made in the form of inner shell and valence shell, and so the W_i values are calculated using the W_i values of the elements that make up the composite (Lee *et al.,* 1990; Akar, 2005).

When a positron of energy and momentum (E, **p**) interacts with an electron that is at first free and idle the positron transfers **q** amount of momentum to the electron and loses W amount of energy. In this situation the W energy transfer corresponding to the transferred **q** momentum is a singular value (Taxiarchis, 2008). The arriving positron then scatters with $\mathbf{p}' = \mathbf{p} - \mathbf{q}$ momentum, $E' = E - W$ energy and $\theta_1$angle of deflection. The target electron possesses recoil energy known as Q energy, **q** momentum and θ_2 angle of deflection. However, in positron-electron interaction when the electron is attached to an atom the transfer of **q** momentum affects the entire atom. Here, as the electron is orbiting the nucleus and is bound to it, the W energy picked up by the electron we get in return for the transfer of q *momentum is not going to be a single value* (Taxiarchis, 2008). In instances such as these the quantities take on random values and are defined by specific probability density functions. In calculations the use of Q recoil energy to replace θ has been adopted and the following equations are used (Negreanu *et al.,* 2005):

$$q^2 = p^2 + p'^2 - pp'\cos\theta \quad \text{and}$$

$$Q = \frac{q^2}{2m} \tag{2.5}$$

In cases of inelastic collisions the differential influence cross-section is given as

$$\frac{d^2\sigma}{dQdW} = \frac{\pi e^4}{E}\frac{1}{WQ}\frac{df(W,Q)}{dW} \tag{2.6}$$

where W is energy transfer and Q is the energy for momentum transfer (Inokuti, 1971). This part of the equation $df(W,Q)/dW$ is generalized oscilation power density. This quantity may be accepted as the number of electrons in an atom that has been subjected to energy transfer between W and W+dW for any given Q recoil energy in an inelastic excitation. In the equation for the differential influence cross-section given for atom-positron interaction W can be given in return for a set Q value or various Q values can be given in return for a set W value, and these (Q,W) values constitute a form of surface known as the "Bethe Surface" (Fernandez-Vera, 1995).

Using this information, taking into account the conditions in small and large momentum transfers the differential influence cross-section is given as:

$$\frac{d^2\sigma}{dQdW} = \frac{\pi e^4}{E}\frac{1}{WQ}\frac{df(W,Q)}{dW} \tag{2.7}$$

$$\frac{d^2\sigma}{dQdW} = \frac{\pi e^4}{E}\frac{1}{WQ}\sum_{i=1}^{M} f_i \frac{dg_i(W,Q)}{dW} \tag{2.8}$$

$$\frac{dg_i(W,Q)}{dW} = \begin{cases} \delta(W - W_i) & Q < W_i \\ \delta(W - Q) & Q > W_i \end{cases} \tag{2.9}$$

where $\delta(x)$ is the Dirac Delta Function. The cross-section's definition can be examined under conditions corresponding to resonance-like and free interactions. For interactions that are similar to resonance $Q < W_i$ and $E > W_i$, by making use

of the Dirac Delta Function's properties the W_i, i-nth shell resonance energy is

$$\frac{d^2\sigma}{dQdW} = \frac{\pi e^4}{E}\frac{1}{WQ}\sum_{i=1}^{M} f_i \frac{dg_i(W,Q)}{dW}$$

$$\frac{d\sigma_{Ri}}{dQ} = \frac{\pi e^4}{E}\int_{W_i}^{E}\frac{1}{WQ} f_i \delta(W - W_i)dW$$

$$\frac{d\sigma_{Ri}}{dQ} = \frac{\pi e^4}{E} f_i \frac{1}{W_i Q}$$

$$\sigma_{Ri} = \frac{\pi e^4}{E} f_i \int_{Q_{min}}^{Q_{max}} \frac{1}{W_i Q} dQ$$

$$= \frac{\pi e^4}{E} f_i \int_{Q_{min}}^{W_i} \frac{1}{W_i Q} dQ$$

Here $Q_{max} = W_i$ because in resonance-like interactions the largest momentum transfer must be equal to the resonance energy. Found as:

$$\sigma_{Ri} = \frac{\pi e^4}{E} f_i \frac{1}{W_i} ln\left[\frac{W_i}{Q_{min}}\right] \qquad (2.10)$$

The scatter angle for the positron that is scattered by this type of interaction is calculated using:

$$Q = 2E - W_i - 2\sqrt{E(E - W_i)}cos\theta_1 \qquad (2.11)$$

There can be no scatter angle for an excited electron in this situation.

For free interaction $Q > W_i$ and $Q > W$ and by using the non-relative Rutherford differential influence cross-section for the positron here (Salvat, 2003) the total cross-section for free interaction is

$$\frac{d\sigma_{Si}}{dW} = \frac{\pi e^4}{E} f_i \frac{1}{W^2}$$

$$\sigma_{Si} = \frac{\pi e^4}{E} f_i \int_{W_i}^{E} \frac{1}{W^2} dW$$

$$\sigma_{Si} = \frac{\pi e^4}{E} f_i \left[\frac{E - W_i}{WW_i}\right] \qquad (2.12)$$

calculated.

As the particle entering interaction is a positron the integral upper limit is taken as E (Negreanu, 2005). The scatter angle for the positron that is released after a free-collision type of interaction is calculated as:

$$Q = 2E - W - 2\sqrt{E(E - W)}cos\theta_1 \qquad (2.13)$$

while the scatter angle for the released electron is calculated as:

$$Q = -W - 2\sqrt{EQ}cos\theta_2 \qquad (2.14)$$

is called the oscillation force. The sum rule from Bethe is:

$$\sum_{i=1}^{M} f_i = Z \qquad (2.15)$$

Z is the atomic number (Liljequist, 1984). The mean ionization energy, I, is

$$\sum_{i}^{M} f_i lnW_i = ZlnI \qquad (2.16)$$

(Liljequist, 1984). There is a similar sum rule for molecules:

$$\overline{f_i} = \frac{\sum_j N_j f_{ij}}{\sum_j N_j} \qquad (2.17)$$

(Le et al., 1990). $W_i W_i$ is for molecules while this is used for resonance energies:

$$ln\overline{W_i} = \frac{\sum_j N_{ij} Z_{ij} lnW_{ij}}{\sum_j N_{ij} Z_{ij}} \qquad (2.18)$$

(Lee et al., 1990). The average ionization energy for molecules:

$$ln\bar{I} = \frac{\sum_j N_j Z_j lnI_j}{\sum_j N_j Z_j} \qquad (2.19)$$

For resonance-like interactions the equations per average free path and stopping power are:

$$\lambda_{Ri}^{-1} = \begin{cases} N\frac{\pi e^4}{E}\frac{1}{W_i}\ln\left(\frac{W_i}{Q_{min}}\right) & E > W_i \\ 0 & E < W_i \end{cases} \quad (2.20)$$

$$Q_{min} = \left(\sqrt{E - W_i} - \sqrt{E}\right)^2 \quad (2.21)$$

$$S_{Ri} = \lambda_{Ri}^{-1} W_i \quad (2.22)$$

And for free interactions is:

$$\lambda_{Si}^{-1} = N\frac{\pi e^4}{E}\left[\frac{E - W_i}{W W_i}\right] \quad (2.23)$$

$$S_{Si} = \lambda_{Si}^{-1} W \quad (2.24)$$

Here N is the number of atoms or molecules per volume.

Using these formulas the equations for total inelastic per average free path and stopping power are (Liljequist, 1983):

$$\lambda^{-1} = \sum_{i=1}^{M} f_i(\lambda_{Ri}^{-1} + \lambda_{Si}^{-1}) \quad (2.25)$$

$$S = \sum_{i=1}^{M} f_i(S_{Ri} + S_{Si}) \quad (2.26)$$

3. The Quantities and Calculations used in the modelling of DNA

When using the algorithm detailed above information such as the atomic weight defining the characteristics of the medium that the positron is going to interact with, the atomic number and density along with the atom shell structure used in the modelling of the atomic formation and the shells' resonance energies all need to be obtained or calculated using appropriate methods. For compound targets in particular, the molecular weight, molecule shell resonance energy, and the intensity of molecule shell oscillation all need to be calculated.

The example calculations below are given for the compound Polymethylmethacrystlate (PMMA - $C_5H_8O_2$):

H $1s^1$

C $1s^2$ $2s^2$ $2p^2$

O $1s^2$ $2s^2$ $2p^4$

If you look at this configuration it will be seen that the inner shells are only valid for the C and O atoms. H only has one electron and this is accepted as an outer electron. Therefore:

For the inner shell : $\bar{f}_1 = \frac{0*8+2*5+2*2}{8+5+2} = \frac{14}{15} = 0{,}93$

For the outer shell : $\bar{f}_2 = \frac{1*8+4*5+6*2}{8+5+2} = \frac{40}{15} = 2{,}67$

0.93 + 2.67 = 3.60 and this value does not give the total number of electrons in the molecule. It does give the ratio by which the electrons are distributed between the inner shells and the outer shells. According to this, if the total number of electrons in the molecule is 15 then:

$$f_1 = \frac{15{,}00}{3{,}60} * 0{,}93 = 3{,}875$$

$$f_2 = \frac{15{,}00}{3{,}60} * 2{,}67 = 11{,}125$$

$$f_1 + f_2 = 3{,}875 + 11{,}125 = 15 = Z_{molecule}$$

Table 1. Resonance energy of some atoms (Akar, 2005).

Atom	W_{inner}(eV)	W_{outer} (eV)
H (Hydrogen)	-	19,19
C (Carbon)	705,23	34,61
O (Oxygen)	898,54	51,58
N (Nitrogen)	941,14	41,077

If the values in Table 1 are used to calculate the resonance energies of the inner and outer shells:

$$ln\overline{W}_{inner} = \frac{N_1Z_1lnW_1+N_2Z_2lnW_2+N_3Z_3lnW_3}{N_1Z_1+N_2Z_2+N_3Z_3} \quad (3.1)$$

$$ln\overline{W}_{inner} = \frac{(8*0*ln(19,19))+(5*4*ln(705,23))+(2*6*ln(898,54))}{(8*0+5*2+2*2)}$$

$$ln\overline{W}_{inner} = \frac{92,7883}{14}$$

$$\overline{W}_{inner} = 755,77\ eV$$

$$ln\overline{W}_{outer} = \frac{(8*1*ln(19,19))+(5*4*ln(34,163))+(2*6*ln(51,58))}{(8*1+5*4+2*6)}$$

$$ln\overline{W}_{outer} = \frac{141,5756}{40}$$

$$\overline{W}_{outer} = 34,45\ eV$$

In Table 1 in the essay by Lee et al. (1990) the K level for PMMA is given as 758eV and the L level is given as 28eV. If compared with this study's findings the results are more or less equal.

Using these values the average ionization energy for PMMA ($C_5H_8O_2$) is:

$$ln\bar{I} = \frac{\sum_j N_jZ_j lnI_j}{\sum_j N_jZ_j} \quad (3.2)$$

$$ln\bar{I} = \frac{5*6*ln78+8*1*ln19,20+2*8*ln95}{5*6+8*1+2*8}$$

$$I = 67,2eV$$

Here, the average ionization energies for Hydrogen $I_H = 19,20eV$, for Carbon $I_C = 78eV$ and for Oxygen $I_O = 95eV$ were taken from the PEGS4 charts. This value that has been found is more or less equal to the value I=65.6eV in the essay by (Lee *et al.,* 1990).

The characteristic values calculated for the compounds used as targets in this study are listed in Table 2.

Table 2. The characteristic values of the composite structure used as the target program of simulation.

Molecule Name	Molecule Weight	Shell Number	f_1	f_2	W_i (eV)	W_v (eV)
Water	18,0105	2	0,666667	2,66667	898,54	40,283
Guanine	151,0491	2	1,375000	3,50000	821,98	36,82
Adenine	135,0541	2	1,333333	3,33333	814,69	35,36
Cytosine	111,0431	2	1,230770	3,23077	809,99	36,13
Thymine	126,0428	2	1,200000	3,20000	793,52	36,61

4. The Monte-Carlo Algorithm for Positron-DNA Interaction

Particles undergoing interaction scatter at different angles. Even if the scatter angles can be calculated using the simulation program that is used, then particularly when a simulation for DNA components is being made the β^+ is accepted as being inside the target and the direction for the released positron is ignored.

The total cross-section for both elastic (E) and inelastic (EO) interactions is written as

$$\sigma_T = \sigma_E + \sigma_{EO} \quad (4.1)$$

For an elastic collision the P_Ω probability of a positron scattering into a solid angle Ω is

$$P_\Omega = \frac{1}{\sigma_E}\int \frac{d\sigma_E}{d\Omega}d\Omega \quad (4.2)$$

Here, if the integral is taken and a correction made using the definition for a solid angle you get;

$$cos\theta = 1 - \frac{2\eta P_\theta}{1+\eta-P_\theta} \quad (4.3)$$

The θ scatter angle for a single elastic collision can be determined using a uniform distribution random number $R_1 \in (0,1)$ instead of probability P_θ:

$$cos\theta = 1 - \frac{2\eta R_1}{1+\eta-R_1} \quad (4.4)$$

The azimuth scatter angle for a positron that scatters following an elastic collision is determined using another number chosen at random $R_2 \in (0\,,1)$ resulting in:

$$\phi = 2\pi R_2 \quad (4.5)$$

The cross-section for inelastic collisions can be written as the sum of the total cross-sections for free interaction (S) and resonance-like interaction (R): If the total cross-section for the collision $\sigma_{EO} = \sigma_R + \sigma_S$ is written again $\sigma_T = \sigma_E + \sigma_R + \sigma_S$.

First of all, the equation

$$P_1 = \frac{\lambda_E^{-1}}{\lambda_T^{-1}} \quad (4.6)$$

is used to determine if the collision is elastic or inelastic. This equation gives the probability (P_1) of the interaction possessing an σ_E elastic cross-section. In this situation, with the aid of a computer generating a random number between $0 < R_1 < 1$ and comparing this number with P_1 it can be decided if the collision was elastic $P_1 < R_1$ or inelastic $P_1 > R_1$.

If the collision is elastic then as there is no energy loss only the positron's change in direction is observed. If it is decided that the collision was inelastic attention is paid to whether the interaction was a resonance-type or a free-type. In order to do this, the probability of it being a resonance-type interaction is calculated using:

$$P_2 = \frac{\lambda_R^{-1}}{\lambda_{EO}^{-1}} \quad (4.7)$$

If by comparing it with a random number matching the condition $0 < R_2 < 1$ if $P_2 < R_2$ it is decided that the collision will be a resonance-type; if $P_2 > R_2$ it is decided that the collision will be a free-type one. Then it needs to be decided if the interaction is going to be with what δ oscillation using model language or with which atom electron from which shell. In this case using

$$P_{Rj} = \frac{\lambda_{Rj}^{-1}}{\lambda_R^{-1}} \quad (4.8)$$

the probability values to be obtained are compared with a random number $0 < R_3 < 1$ that is determined by computer. However, as more than two options can arise the calculation is edited a little: It may be written as

$$P_j = \frac{\lambda_j^{-1}}{\lambda^{-1}}; \qquad \sum_{j=1}^{M} P_j = 1 \quad (4.9)$$

and when making the decision the formula:

$$P_1 + P_2 + \ldots + P_{j-1} \equiv A_{j-1} < R_3 < A_j \quad (4.10)$$

may be used.

The average free path is inversely proportional to the cross-section. However, the path taken between two interactions exhibits deviation from the average and may be exemplified in the form

$$\text{path lenght} = -\lambda \ln(1 - R_4) \quad (4.11)$$

by using a random number $0 < R_4 < 1$. The average result obtained from a sufficiently high number of samples converges to the value λ.

During the simulation in resonance-type interactions when sampling the positron's energy loss it is sampled as the difference between the energy levels determined by the rules of quantum physics depending on the target's makeup. As the target is at ground level the excitation will be at the highest vacant energy level. In free-type interactions the sampling of the energy loss is determined as the ionization energy of the ionized electron plus kinetic energy and the difference in kinetic energy imparted to an electron in this state is the reason why the positron's energy loss is different. The greatest energy that can be imparted to the target electron is the kinetic energy possessed by the positron. The average energy loss obtained as a result of multiple repetitions of free-type interactions converges either from the left or from the right of the value $W_{average}$.

The target's stopping power S is defined as the energy lost by the positron per path length

between the two interactions. However, this quantity is an average value and is calculated by dividing the average values of the amount of energy lost and the path taken between the two interactions by one another. In order for these values to achieve a sound result it is necessary to take a large number of values and calculate the average. In this study every calculation was the result of more than 25,000 outcomes. In some cases, it was necessary to use 40,000-50,000 outcomes:

$$\langle S \rangle = \frac{E_{average}}{\lambda_{average}} \qquad (4.12)$$

5. Results and Discussion

Water was primarily used as the target medium to test the Monte-Carlo simulation program developed in this study.

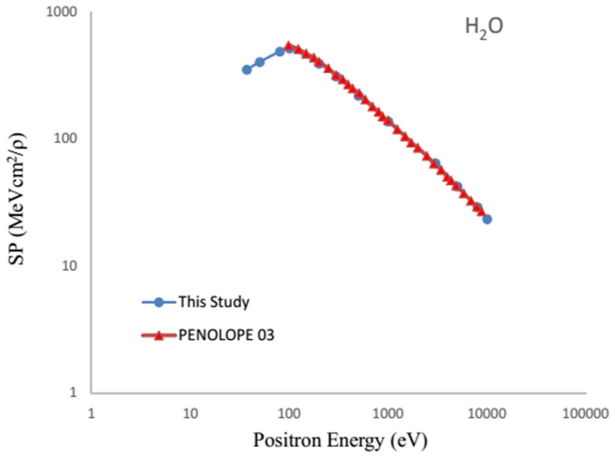

Figure 1. The mass stopping power of liquid water. The results of PENELOPE03 were taken from the paper by Gümüs *et al.,* 2006.

In Figure 1 it can be seen the comparison of the stopping power obtained for water with the results presented by the PENELOPE 03 code of the graphic drawn for positron energies. The maximum value of the stopping power (518.72MeVcm²/ρ) was found to be approximately at 100 eV and this value matched the value obtained using the PENELOPE03 code. While this study is able to calculate the stopping powers for positron energies less than 100eV, PENELOPE03 gives the results for energies larger than 100eV. In ICRU Report 37 the stopping power values begin at 10keV with the value given for 10keV being 24.83MeVcm²/ρ. In this study the value found for 10keV is 23.50MeVcm²/ρ . The results are compatible having a 5% difference. Similarly, the study for positrons made by Tanır at al. (2012) found the maximum stopping power (416.79MeVcm²/ρ) to be approximately 100eV using a calculation known as SP2. In that same study's comparisons in Figure 1 you can see the work in the low energy region that could not be calculated.

The stopping powers corresponding to positron energy of guanine ($C_5H_5N_5O$), adenine ($C_5H_5N_5$), thymine ($C_5H_6N_2O_2$) and cytosine ($C_4H_5N_3O$) are given in Table 3. The maximum stopping power was found at around 80eV of positron u the stopping power of low positron energies. The ability to determine the stopping power for positrons that have slowed to the eV range is vitally important for being able to calculate correct radiation dosage. In 2005, Akar and Gümüş calculated the stopping powers of these four nucleotides for electrons. Even though there are differences in how electrons and positrons interact with the target their comparison is significant in terms of being able to be calculated in low energy ranges. They reported that the maximum stopping power for all of them was at 80eV and they gave the following results: 371.25 (adenine), 356.3 (guanine), 370.84 (cytosine) and 367.95 (thymine) MeVcm²/ρ. In this study the results were 498 MeVcm²/ρ for adenine, 477.68 for guanine, 504.27 for cytosine and 495.24 for thymine. It can be said that the reason for the differences is from the differences between in how the positrons and electrons interact with the target. In ICRU Report 37 the water's stopping power for electrons at 10keV is seen as 22.57 MeVcm²/ρ and 24.83 MeVcm²/ρ for positrons. The difference is approximately 10%. The DNA chain at the cell's nucleus is made up of Adenine, Guanine, and Cytosine and Thymine molecules in the following ratios: Adenine 29.3%, Guanine 20.7%, Cytosine 20% and Thymine 30% (NIST). The data for these molecules' stopping power for positrons is given in Table 3. In the interaction between DNA and positrons it is possible to make a rough calculation of DNA's stopping power by using the percentages of the component molecules found in the DNA. The result of these calculations is given in Table 3 and plotted in Figure 2 and Figure 3.

Table 3. The mass stopping powers of H_2O, guanine, adenine, thymine, cytosine, DNA and Cell for positrons with low energy SP/ρ (MeVcm²/ρ).

E (eV)	H_2O	Guanine	Adenine	Thymine	Cytosine	DNA	Cell
10000	23,50	21.07	21,50	22,01	21,03	21,47	22,99
8000	29,15	25.52	27,00	26,86	28,15	26,88	28,58
5000	42,37	40.51	38,70	39,42	39,22	39,39	41,63
3000	64,56	55.09	59,20	60,04	58,05	58,37	63,01
1000	137,89	122.71	121,00	124,57	124,91	123,21	134,22
500	220,48	193.66	194,00	194,16	195,69	194,32	213,94
300	310,69	266.51	271,00	275,24	272,63	271,67	300,93
200	393,56	337.20	344,00	351,57	348,58	345,78	381,61
100	518,72	456.70	473,00	473,55	476,66	470,52	506,67
80	490,26	477.68	498,00	495,24	504,27	494,22	491,25
50	405,20	416.90	453,00	433,70	444,88	438,11	373,89
37	352,48	56.01	185,00	87,55	133,15	118,69	294,03

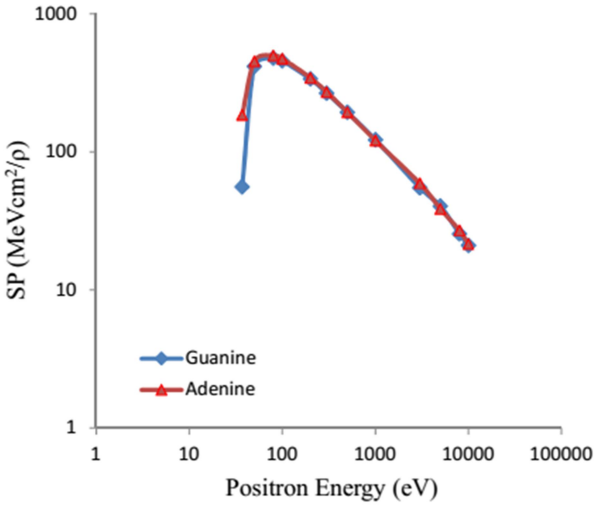

Figure 2. The stopping powers of guanine and adenine.

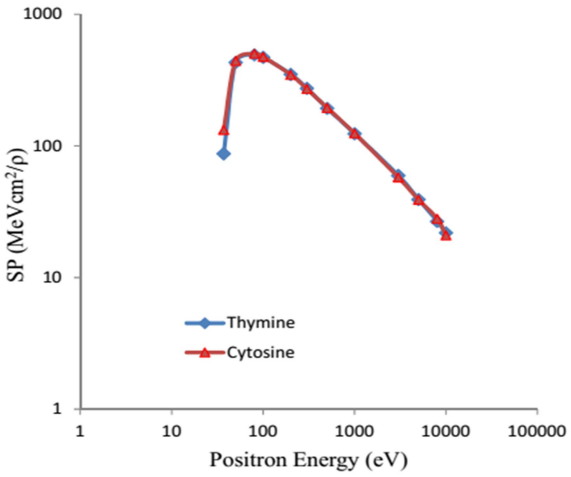

Figure 3. The stopping powers of thymine and cytosine.

Given that roughly 75% of the cell is water and 25 percent is DNA the cell's stopping power for positrons in the interaction was calculated using both water's and the DNA's stopping power values. The data for one cell are given in Table 3 and plotted in Figure 4. In the study by Tufan et al (2013) the stopping power of brain tissue for positrons was calculated for the 100eV - 1MeV range. At 100eV the maximum stopping power was calculated as 332.37 MeVcm²/ρ. When compared with the values found for the cell in this study it can be seen that the maximum SP fits the observed positron's energy. However, there are no results for energies lower than 100eV.

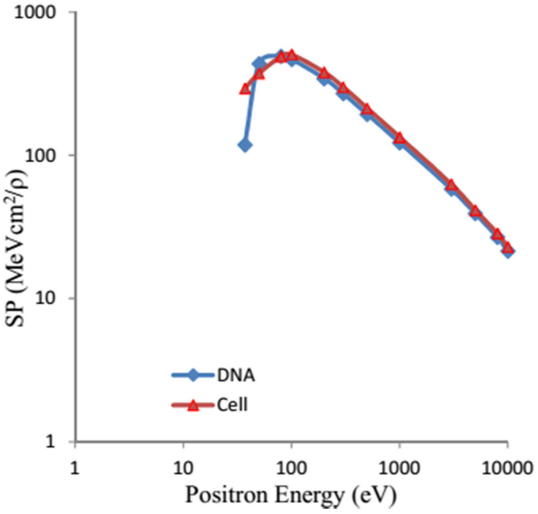

Figure 4. The mass stopping powers versus positron energies in a cell and DNA.

As can be seen in Table 3, the maximum stopping power is 494.22 MeVcm^2/ρ for DNA at 80eV and 506.67 MeVcm^2/ρ for the cell at 100eV. No comparison was made with the values for targets at low energies given in other studies. However, the results do fit with existing comparisons and so it can be said that the findings obtained for DNA and the cell are matching results.

6. Conclusion

In this study stopping power values for positrons with low energies in biological materials were determined using the Monte Carlo simulation. One key advantage of the Monte Carlo simulation is that it allows SP values to be determined for energy levels lower than 100eV. The results of this study found using Monte Carlo were obtained using analytical calculation and significant differences with respect to SP scales were found when compared with other studies. There is no difference in SP values' corresponding energies. This is quite important for the planning of dosage in radiation oncology, nuclear medicine and even fields were gamma-knife is used.

It can be concluded that the energy of incident particles to the target material is a key parameter in determining stopping power. It has to be noted that stopping power must be known accurately in order to determine the radiation dose that is given to the patient.

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