Calculation Of WER And WET For 3 Dosimetric Materials At Carbon Ion Energies Ranging 100-300 Mev Using Fluka And MCNPX Monte Carlo Codes

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Calculation of WER and WET for 3 dosimetric materials at carbon ion energies ranging 100-300 MeV using Fluka and MCNPX Monte Carlo codes

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Abstract: Due to the shortage of data regarding range, WER and WET values for carbon ion beams in a vast range of energies as well as for relevant dosimetric materials, in this work, firstly, depth-dose profiles and range were evaluated in liquid water, polyethylene (PE), aluminium, bone, polymethyl methacrylate (PMMA), and lead for carbon ion energies ranging 100-300 MeV using Fluka Mc code. Afterwards, following their most frequent use in dosimetric studies in hadrontherapy, we decided to calculate the WER and WET of only 3 dosimetric materials (PE, PMMA and lead). Then, we made the remark that the PE and the lead represent the least and the most difference to water with calculated mean WER values of 0.998 and 5.684, respectively. The calculated WER values were compared with MCNPX Mc code as well as the previous analytical results (NM, BK, BB, EBB). Good agreement was reached between Fluka, MCNPX and the previous analytical results. The largest discrepancy between the two Mc codes was 2.29% for lead at 250 MeV carbon ion energy and was about 2.06% between Fluka and the BB method for Lead at 270.83 MeV carbon ion energy . Based on the materials explored, the PE stayed the nearest to water with an average WER of 0.9983 for carbon ion energy ranging 100 to 300 MeV.

KeysWords: WER, WET, carbon ion, hadrontherapy, Fluka, MCNPX

1 Introduction

Since the discovery of X-rays, radiation has been used to treat different diseases such as cancer. [1] . From that time, a lot of studies have been executed to enhance radiotherapy outcomes, in which the radiation is accurately targeted at tumors to allow a greater uniform dose while diminishing harm to nearby normal tissues and organs. In this regard, the use of the carbon ion beam as a new type of radiation is a method that has been introduced to the domain of radiotherapy recently, and it is unique and has multiple physical and biological advantages without forgetting the effect of their secondary particles on the surrounding tissues which prevents until now a great investissement on it.[2] Charged particle beams that impinge on the body, especially the carbon ion beam, deposit energy along their ways[3] . The depth of penetration of the particles in the thick of the body is set by their acceleration energy, and charged heavy particles in the style of carbon ions deposit more energy the deeper they go into the body rising to a high peak at the end of their range (where the residual energy is lost over a very short distance). This results in a sharp rise in the absorbed dose, known as the Bragg peak. After the Bragg peak, there is a rapid drop-off of the dose to roughly zero for the carbon ion beam. The use of carbon ion radiation therapy in medical practice is anchored on appropriate calibration to preserve human organs and tissues. Few years ago, it was impossible to directly control the dose distribution in patients treated with any type of radiation [4]. Nowadays, positron emission tomography (PET) and prompt gamma imaging (PGI) are two promising modalities for range verification. However, the relatively long acquisition time of PET and the relatively low yield of PGI pose challenges

for real-time range verification [5]. The data on the dose distribution are entirely obtained from measurements in phantoms constructed from tissue equivalent materials. In clinical carbon ion dosimetry, the measured dose distribution data are usually procured in a liquid water phantom which has similar properties to soft tissue. However, water phantom has many disadvantages when utilized in conjunction with detectors[6]. Various water equivalent solid phantoms have been introduced as substitutes for water in the measurement of the absorbed dose. For a specific material to be tissue or water equivalent, it must have the very same mass stopping power and secondary particle production, electron density, effective atomic number and mass density like water. A carbon ion range, which was quantified for the chosen material and liquid water, is utilized as an equivalence estimator. For this purpose, the parameters of both the water equivalent ratio (WER) and the water equivalent thickness (WET) were taken into account to compare the dosimetric equivalency of the materials with water. Several theoretical and numerical works were undertaken to promote the calculation of these quantities in a large range of materials. Zhang and Newhauser used the numerical method [NM] presented by Newhauser et al. to calculate WER values for some materials [7].Also, in another work, Zhang et al. [8] estimated analytical values of the WER for some opted materials utilizing the Bragg–Kleeman [BK] rule. This approach was also employed by Zhang and Newhauser [7]. The BK rule determines the range of the carbon ion beam in specified materials employing two materials and energy-dependent constants.

Note that for proton therapy most of the calculations of WER and WET were made, namely theoretical, experimental and numerical ones for a large range of proton energy [9]. Contrary to that and according to our good understanding of carbon-therapy, theoretical calculations of WER and WET ,which were made only for some dosimetric materials, were the only ones that were found. [7]. In addition to that, WET of these materials is calculated for very little thickness. Therefore, in this work and based on Fluka Mc code version 2020.0.beta [10][11], we calculated the range of carbon ions in 6 dosimetric materials and then we chose to calculate the WER of PE, PMMA and Lead following their most frequent use in dosimetric studies in hadrontherapy. Also, the energy interval was fixed between 100 to 300 MeV with a step of 50 MeV. Then, we tried to compare our calculations with those obtained by the MCNP code and the old theoretical studies (NM, BK, BB, EBB).

Moreoever, we still calculated the WET of the studied materials for PMMA and PE of 5 and 10 cm and for lead of 5 and 2.5 cm. Good agreement was observed between our calculations and comparable calculations.

2 Materials and methods

2.1 WER and WET

Particle range is the distance travelled by a particle while penetrating an absorber before losing the totality of its energy and stopping completely. Particle range is reliant on energy ,particle type and absorber material. The Continuous Slowing Down Approximation (CSDA) range, is the range of an ideal particle experiencing always the average energy loss and no angular deflection[12]. The depth dose curve, involving the Bragg peak, for a monoenergetic carbon ion pencil beam in a homogenous liquid water phantom is given in figure 1. The clinical range of carbon ion beam (R) is outlined as the distal depth to the Bragg peak where the dose is decreased to 80% of its maximum Bragg peak value. If a flat slab of thickness, tm, of certain non-water material is now placed in front of the water phantom, and again the same monoenergetic carbon ion beam is incident on its surface, the $R^{W}_{80\%}$ will shift backwards/forwards by WET of tm ($R^{W.Sh}_{80\%}$). Thus, WET here is stipulated as [13] :

$$WET = R^{W}_{80\%} - R^{W.Sh}_{80\%} = tm\frac{\rho_m}{\rho_w}(\frac{s}{\rho})^{m}_{w} \qquad (1)$$

where:

-$R^{W.Sh}_{80\%}$: the resultant clinical carbon ion range due to the presence of a slab tm [cm].

-ρ_m and ρ_w: the densities of the slab and water [g/cm^3], respectively.

-$(\frac{s}{\rho})^{m}_{w}$: the ratio of carbon ion mass stopping power of the slab over water.

Three approaches were employed to calculate the mean mass stopping power in the material of interest based on relationships between theoretical

mass stopping power and beam energy. The first relationship is based on the Bragg–Kleeman (BK) rule (Bragg and Kleeman 1905):

$$S = \frac{E^{1-p}}{\alpha \rho p} \tag{2}$$

where α and p are material-dependent constants and E is the initial energy of the heavy charged particle beam. The values of α and p were acquired by fitting to either residual ranges or stopping powers data (Ziegler et al 1985). A second relationship between range and energy for heavy charged particle beams is captured in the Bethe–Bloch (BB) equation (Bethe 1930, Bloch 1933):

$$S = 4\pi N_A r_e^2 m_e c^2 z^2 \frac{Z}{A}\frac{1}{\beta^2}[\ln \frac{2m_e c^2 \gamma^2 \beta^2}{I} - \beta^2 - \frac{\delta}{2} - \frac{C}{Z}] \tag{3}$$

where N_A is Avogadro's number, r_e is the classical electron radius, m_e is the mass of an electron, z is the charge of projectile, Z is the atomic number of the absorbing material, A is the atomic weight of the absorbing material, c is the speed of light, $\beta = \nu/c$ where ν is the velocity of the projectile, $\gamma = \frac{1}{\sqrt{1-\beta^2}}$, I is the mean excitation energy of the absorbing material, $\frac{\delta}{2}$ is the density effect correction and $\frac{C}{Z}$ is the shell correction.

The Barkas effect, associated with a z^3 correction to the stopping power, is well pronounced at low energies. The correction is due to target polarization effects for low-energy distant collisions and can be accounted for by the following expression [14]:

$$L_0(\beta) + \frac{\delta}{2} \longrightarrow (L_0(\beta) + \frac{\delta}{2})(1 + 2\frac{z}{\sqrt{Z}}F(V)) \tag{4}$$

where $V = \frac{\beta\gamma}{\alpha\sqrt{Z}}$. The function F(V) is a ratio of two integrals within a Thomas-Fermi model of the atom.

The Bloch correction should also be taken into account. L_{Bloch} is the stopping number, and the standard expression of Bloch's formula is summed up in the following equation [15]:

$$L_{Bloch} = \psi(1) - Re[\psi(1+iy)] = -y^2 \Sigma_{j=1}^{\infty} \frac{1}{j(j^2+y^2)} \tag{5}$$

where ψ is the logarithmic derivative of the Γ function, and $y = z\frac{\alpha}{\beta}$($\alpha = 1/137.036$ is the fine structure constant).

At low projectile velocities, the effect of the partial neutralization of ions towards the end of their range and loss due to interactions with target atoms -the so called z_{eff} parameter- should be taken into account as well.

For compounds and mixture materials, the mass fractions of each constituent element are needed to calculate the effective atomic number Z_{eff} and the effective atomic weight A_{eff}, for the mixture as

$$Z_{eff} = \sum_i a_i Z_i \tag{6}$$

$$A_{eff} = \sum_i a_i A_i \tag{7}$$

respectively, where a_i and Z_i are the relative number of moles of element i per mole of compound and the atomic number respectively (Leo 1987). We previously proposed an empirical formula to calculate I in an empirical form of the BB equation (EBB) (Zhang and Newhauser 2009), such that $I = kZ$, where $K = 14.5$ when $Z \leq 8$, $K = 13$ when $8 < Z \leq 13$ and $K = 11$ when $Z > 13$. An iterative NM of WET calculation described by Newhauser et al (2007a) was used as one of the standard of comparison for the other analytical formulas used here, because it is the most exact one of the methods considered.

It is convenient to use the water equivalent ratio (WER) concept, in clinical practice, in representing the difference between the practical range of carbon ions in water ($R^W_{80\%}$) over the practical range of carbon ions in a certain material m, ($R^M_{80\%}$) (Andreo et al 2000, Zhang et al 2009, 2010, Vera et al 2014). WER is defined as:

$$WER = \frac{R^W_{80\%}}{R^M_{80\%}} \tag{8}$$

2.2 Simulation

2.2.1 Fluka MC code

In this study, we modeled a target geometry using Flair 2.3-0 [16] (FLUKA 2020.0.beta Advanced Interface).It is in the form of a cylinder with a height of 30 cm and a 10 cm radius surrounded by a vacuum sphere which itself is surrounded by a black hole sphere (a material that gives an end to the

course of the particles which cross it by their absorption).
This cylinder is filled by a precise phantom each time we want to calculate the range of the incident carbon ions. first, the range was calculated in 6 dosimetric phantoms for a multienergetic beam ranging from 50 to 300 MeV of the carbon ions. Then, we focused only on 3 dosimetric phantoms (PMMA, PE, LEAD) following their major uses in hadrontherapy by calculating their WERs. Table 1 presents the properties of the investigated dosimetric materials. Recently, the I value of water has been changed to 78 eV instead of 75 eV, and this should be taken into consideration when dealing with the results of this study. FLUKA simulations were carried out using the recommended parameters "HADRON THERAPY" and take into account :

- inelastic form factor corrections to Compton scattering and Compton profiles.
- electromagnetic interactions, manipulated by the ElectroMagnetic Fluka (EMF) package that administers energy loss, straggling, and multiple Coulomb scatterings of charged particles.
- low-energy neutron transport down to thermal energies.
- Entirely analog absorption for low-energy neutrons.
- particle transport threshold fixed at 100 keV, except for neutrons (10^{-5} eV).
- multiple scattering threshold at minimum permitted energy, for both primary and secondary charged particles.
- hadron-nucleus interactions, described by the PEANUT model.

Furthermore, we offered new results about the WET of the studied dosimetric materials for different thicknesses and also for a carbon ion beam ranging from 100 to 300 MeV with a step of 50 MeV. For this purpose, we used a parallelepiped of varying thicknesses filled each time with the phantom to be studied, which was centered by the same axis as that of the cylinder and placed before it. In this work, WET is calculated based on equation 1 and WER is calculated using equation 7.

2.2.2 MCNPX

To validate our calculations, we used the MCNP cross-section by application of ENDF/B-VII.
There are many scientific studies that have been done following the interactions between particles and matter using MCNP. Based on MCNPX 2.7.0 [17], the target was simulated as a cylinder volume which is surrounded by air with the axis of symmetry in the direction of propagation of the incident beam. The dimensions of that target were 30 cm heightwise and 5 cm in terms of radius. The region of the air surrounding the target had a length of 60 cm and a radius of 25 cm.
In this simplified model, the total energy deposition was noted in cells of 0.01 cm width in the direction of the incident beam. The calculation ,which was made by Fluka Monte Carlo code, is redone for a purpose of validation by MCNPX for the studied energies.

3 Results and discussion

In figure 1, depth dose distributions were calculated for 6 dosimetric materials for an energy interval of carbon ions that goes from 50 to 300 MeV. It was found that the greater the beam energy is, the deeper the maximum deposited dose is.

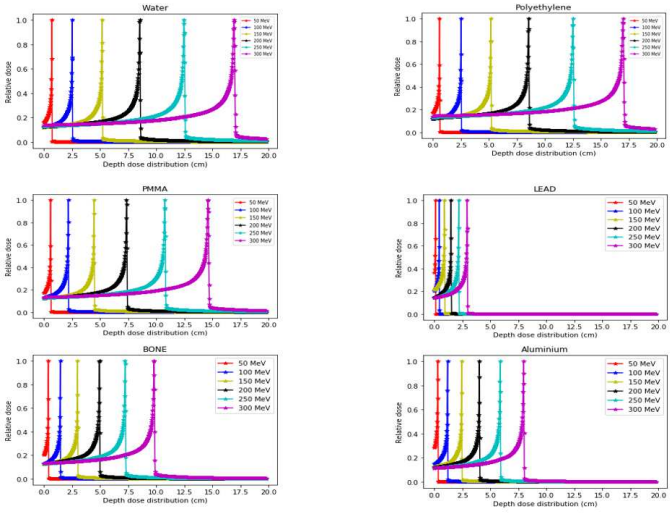

Figure 1: Calculated depth dose distributions for the studied materials for selected carbon ion energies. Data are normalized to the dose of the Bragg peak.

Table 1: Chemical formula, density (g/cm^3) and excitation energy (eV) for the discussed materials

Materials	chemical formula	ρ(Fluka)	ρ(MCNPX)	ρ(NM,BK,BB,EBB)	$< I >$
Water	H_2O	1	1	1	75
PE	$(CH_2)_n$	0.94	0.94	0.964	57.4
PMMA	$(C_5H_8O_2)_n$	1.19	1.19	1.185	74
Lead	Pb	11.35	11.30	11.322	823

To compare the Bragg peak position of the studied materials for the same carbon ion beam energy, the depth dose profiles are given in figure 2 for 300 MeV carbon ion beam. It is necessary to note that the materials with lower density produce longer range due to lower stopping powers.

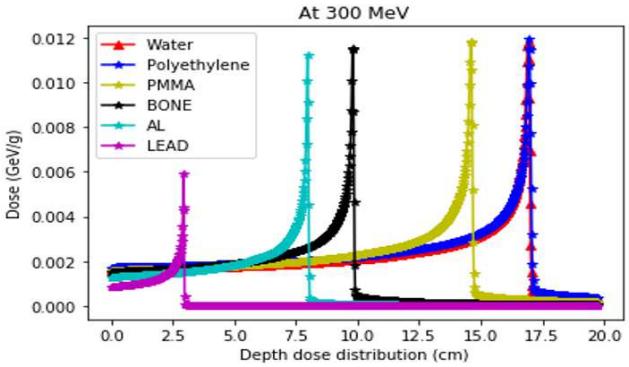

Figure 2: Depth dose distribution of the studied materials for 300 MeV carbon ion beam

In the figure above, one can easily notice that for a given carbon ion beam energy, the largest differences in the Bragg peak position with respect to liquid water are observed in lead and aluminium. Moreover, the results for polyethylene (PE) present the most analogous depth dose characteristics to liquid water as an available dosimetric phantom which is close to muscle and other soft tissue.

The range values of the studied materials obtained using the Fluka Mc code are shown in table 2 for the studied carbon ion energies.
Figure 3 represents the difference between the ranges of carbon ions in water and the investigated dosimetric materials versus the carbon ions energy based on the results of table 2. As long as the energy of the carbon ions increases, this difference becomes larger. Generally, polyethylene and lead have the smallest and largest range difference relative to water.

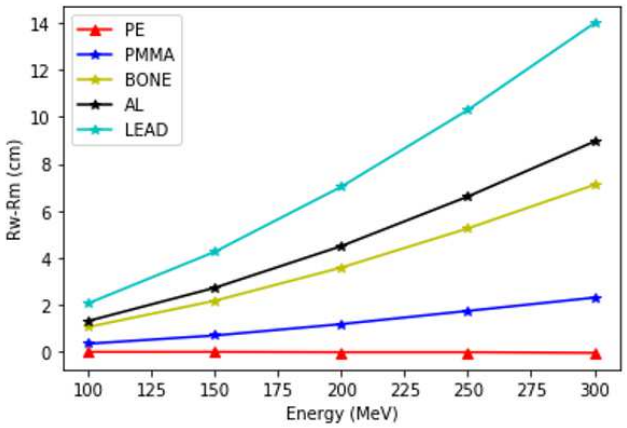

Figure 3: Differences between carbon ion range in water (Rw) and studied dosimetric materials (Rm) versus carbon ion energy.

At times, the PMMA and PE are preferred (convenience included) instead of water for dose measurements. Additionally, solid materials such as the PMMA, PE and aluminium frequently (partly) make up the composition of dosimeters (Andreo et al 2000, Fellin et al 2017). Thus, conversion factors are often required to calculate dose in water and other biological tissues.
In this study, the WER values were calculated using the two MC codes and were compared to some available previous theoretical calculations (NM,BK,BB,EBB) for 100-300 MeV carbon ions beam .These ones are presented in table 3.

Additionally, Fluka and MCNPX calculations of WER are shown in figure 4 where previous analytical results (NM,BK,BB,EBB) are presented, but this time just for the PMMA and the PE ranging 100-300 MeV carbon ion beam. In general, the WER values are quite dependent on the slab material, thickness, compositions, excitation energy values and carbon ion energy. For example, the WER values were greater for higher density materials for a given energy, while they were largely independent of energy for lower density materials. The WER

Table 2: Fluka data of carbon ion range (cm) for studied materials at different carbon ion energies

Materials	100MeV	150MeV	200MeV	250MeV	300MeV
Water	2.5188	5.1801	8.5403	12.492	16.927
PE	2.5188	5.1801	8.5538	12.505	16.968
PMMA	2.1694	4.4812	7.3575	10.747	14.616
Bone	1.457	3.0027	4.9516	7.2366	9.8172
Aluminium	1.2016	2.4516	4.0376	5.879	7.9758
Lead	0.4489	0.91935	1.5108	2.1962	2.9355

Table 3: WER of the studied materials at different carbon ion energies

Dosimetric material	method	Carbon ion energies (MeV)								
		100	150	187.5	200	229.17	250	270.83	291.67	300
PMMA	Fluka	1.161	1.1559	1.159	1.1607	1.1591	1.1623	1.1569	1.1589	1.1581
	MCNPX	/	1.1331	/	/	/	1.1563	/	/	/
	NM	/	/	/	/	/	1.157	1.158	1.157	/
	BK	/	/	/	/	/	1.158	1.158	1.158	/
	BB	/	/	/	/	/	1.167	1.167	1.166	/
	EBB	/	/	/	/	/	1.159	1.158	1.158	/
PE	Fluka	1	1	0.9982	0.9984	0.9975	0.9989	0.9972	0.9974	0.9975
	MCNPX	/	1.001	/	/	/	1.002	/	/	/
Lead	Fluka	5.6107	5.6345	5.6612	5.6528	5.7082	5.6880	5.6941	5.742	5.7663
	MCNPX	/	5.690	/	/	/	5.8219	/	/	/
	NM	/	/	5.57	/	5.675	5.712	5.743	5.771	/
	BK	/	/	5.583	/	5.684	5.720	5.749	5.776	/
	BB	/	/	5.647	/	5.754	5.787	5.814	5.836	/
	EBB	/	/	5.568	/	5.679	5.713	5.741	5.764	/

Table 4: WET of the studied materials for different thicknesses and at several carbon ion energies

Dosimetric material	T (cm)	Carbon ion energies (MeV)				
		100	150	200	250	300
PMMA	5	5.3279	5.67069	5.7211	5.6741	5.304
	10	10.3535	10.7164	11.1142	11.4705	11.4196
PE	5	4.9751	4.94825	4.9146	4.8677	4.817
	10	10.0309	9.9382	9.9045	9.8576	9.7899
Lead	5	7.0585	9.2493	12.0215	15.2843	18.9633
	2.5	4.5719	6.746	7.56248	12.78098	14.2926

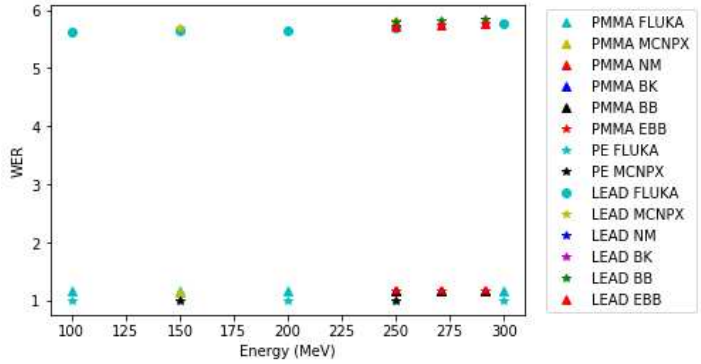

Figure 4: WER distributions for different carbon ion energies in the studied materials.

values were nearly constant between 100-300 MeV range for all materials.

For PMMA, the value of WER increases from 1.1559 at 150 MeV to 1.1623 at 250 MeV. For these two energies, the maximum and the minimum calculation error between Fluka and MCNPX is 2.01% and 0.5% respectively, while it is between 0.03% (EBB) and 0.04% (BB) at 250 MeV between Fluka and the previous theoretical studies.

For the PE, the value of WER decreases from 1 at 150 MeV to 0.9989 at 250 MeV. For these two energies, the maximum and the minimum calculation error between FLUKA and MCNPX is 0.09% and 0.02%, respectively. Concerning the lead, the value of WER increases from 5.6345 at 150 MeV to 5.6880 at 250 MeV. This time, for these two energies, the maximum and the minimum error of calculation between Fluka and MCNPX is 2.29% and 0.09% respectively, while it is between 0.04% (NM) and 1.71% (BB) at 250 MeV between Fluka and the previous theoretical studies. These bi-code fluctuations appear due to different physic approaches implemented in each code which are contributed in by both stopping power and physic approaches. As we noticed from table 3, the maximum deviation of calculations between Fluka and the 4 previous theoretical studies is always between our calculations and the BB method. This maximum deviation occurred because of the difference in density and excitation energy $< I >$ between the two methods.
At the same stage, another conversion factor comes into play; it is the WET.
In this work, we calculated the WET of the 3 dosimetric materials studied for thicknesses of 2.5 cm, 5 cm and 10 cm. For PMMA and PE, due to their low density, we chose to calculate this factor only for thicknesses of 5 cm and 10 cm, but for the lead, which has a high density, this thickness has been reduced a little to 2.5 cm. All these calculations are presented in table 4.

The variation of WET as a function of the energy interval of the carbon ions studied for a fixed thickness of 5 cm for the 3 dosimetric materials is presented in figure 5.

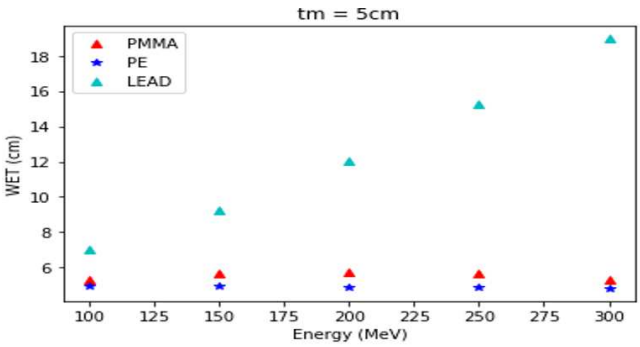

Figure 5: WET of the studied materials for Tm=5 cm at several carbon ion energies

From this figure, we notice that the WET of the lead is greater than that of PMMA and PE for a fixed energy, and this is due to its high density which intervenes in the calculation of this factor (equation 1). It can also be deduced from this figure that this factor is independent of the energy of the incident carbon ions for PE and PMMA, but it is largely dependent on this energy for the lead. This shows that to have the same range in water and in lead for a given energy, a phantom of water that is too thick is required.
Based on our WER and WET calculations and following the advantages they possess, we may well conclude that we can use other phantoms for dosimetry reasons instead of the water phantom.

4 Conclusion

To sum up, in the current work, firstly, range and depth profiles were calculated for 6 dosimetric materials (water, PE, PMMA, lead, aluminium and bone) using Fluka MC code.
Then, due to the lack of data concerning the two conversion factors (WER and WET) for carbon ions we calculated the WER of only 3 dosimetric

materials (PE, PMMA and lead) following their frequent utilzation in hadron therapy for an interval energy goes from 100 to 300 MeV.
Our calculations were in a good agreement with MCNPX (a maximium relative error less than 2.29%) and the 4 previous analytical results (NM, BK, BB, EBB) with a maximum relative error less than 2.06%.
We also calculated WET of the investigated materials for different thicknesses; we concluded, on one side, that WET is greater for the lead than for the other studied materials at a fixed energy. On the other side, we noticed that this factor is independent of the energy of the incident carbon ions for PE and PMMA, but it is predominantly dependent on this energy for the lead.
Finally, based on WER and WET calculations done in this work, PE exhibits least difference to water for carbon ion energy ranging from 100 to 300 MeV.

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