Abstract. It is shown, for the first time in a systematic way, that by employing experimental constraints on the shape parameters of the Bragg peak, along with its position, the accuracy in empirical estimation of the mean ionization potential of the stopping medium can be improved. The particular case considered in the present work has a high relevance for hadrontherapy, namely beams of $^{12}$C ions stopped in water targets. Experimental data at 12 incident beam energies in the range of interest for therapy are compared with the numerical simulations performed with the FLUKA and PHITS computer codes. For each data set a narrow range of values for the mean ionization potential of water is obtained.

Key words: Bragg Peak, Shape parameters, Hadrontherapy, FWHM.

1. INTRODUCTION

Nowadays beams of heavy charged particles (HCP), particularly protons and $^{12}$C ions, have become instruments of clinical applications in radiotherapy [1]. By their use, an innovative tumor treatment method called hadrontherapy has emerged [2]. The "inverse" dose distribution (Bragg curve) of the HCP relative to X-rays and electrons creates a unique means to depose a high dose in a deep seated tumor while minimizing the irradiation of the adjacent healthy tissues [3]. Moreover, the intense ionization density produced by the HCP, particularly in the Bragg peak region, results in a much stronger radiobiological effect than in conventional radiotherapy [4].

At present several treatment centers are in operation worldwide [5], specializing in tumor therapy by proton and carbon energetic beams [6, 7]. Others are either under construction or in planning stages, such as ETOILE in Lyon (France), CNAO in Pavia (Italy), Med-AUSTRON in Wiener Neustadt (Austria) [8]. Intensive research efforts to increase the performances of hadrontherapy
techniques are systematically performed at basic scientific research facilities, e.g. the Heavy Ion Research Center (GSI) in Darmstadt, Germany [7] and the Heavy Ion Medical Accelerator (HIMAC) in Chiba, Japan [9].

For precise determination of the dose delivered by HCP irradiation to biological tissues, extensive experimental tests on water phantoms and numerical simulations must be performed. Moreover, accurate knowledge of the atomic and nuclear processes occurring at the interaction of the HCP with matter and reliable estimates for the values of the interaction parameters (cross sections, ionization energies, etc.) is strongly required [10].

It is the goal of the present work to propose and test a method that improves the accuracy in the empirical estimation of the average ionization potential $\langle I \rangle$ for water. This is an important parameter that has to be provided as input value in any numerical simulation of the HCP stopping in water targets. For the first time a set of three Bragg peak shape parameters are employed along with the Bragg peak position, in order to impose stronger constraints on the $\langle I \rangle$-values that provide good reproduction of the experimental data. Extensive calculations performed with the FLUKA [11] and PHITS [12] transport codes are compared with experimental data both on the Bragg peak position and Bragg peak shape parameters. For comparison with calculations all available experimental Bragg curve data of $^{12}$C ion beams stopped in water, at energies in the therapeutic range were considered.

The mean ionization potential values employed in the present numerical simulations are selected to cover all values previously reported in literature (see Section 2). By including the Bragg peak shape parameters in the analysis, a clear narrowing was obtained for the range of $\langle I \rangle$-values which make experimental data compatible with the calculated ones.

Following a brief description of the HCP stopping process (Section 2), in Section 3 the procedure used to account for the experimental data and for the estimation of uncertainties in the determined Bragg peak shape parameters is thoroughly reported. Section 4 presents the computer codes and the input parameters employed in the numerical simulations and Section 5 is dedicated to an extensive discussion of the comparison between experimental values and numerical simulation results. For each data set a range of $\langle I \rangle$-values providing the best agreement between experiment and theory for all considered observables are determined. Conclusions of the present work are synthesized in the last section.

2. STOPPING POWER OF CHARGED PARTICLES

Dose deposition of energetic ions in matter is proportional to the energy loss per unit path length $- (dE/dx)$ of the projectile particles, known as the stopping power. The main energy loss mechanisms are inelastic collisions with atomic electrons (electronic stopping) and interactions with the target nuclei (nuclear stopping) [13]:
Although the second term is quantitatively less important, it is more difficult to be precisely estimated at the high therapeutic energies, especially when complex projectiles like carbon ions and complex targets like biological tissues are involved. It includes several processes: target and projectile fragmentation, radiation losses, charge exchange between projectile and target, all leading to a time dependent projectile charge and energy transfer to the vibrational and rotational states of the target etc.[14]. In the physical models of stopping which are employed in the transport codes some of these processes are always neglected and therefore differences in results can arise.

Within the range of therapeutically relevant energies 100–400 MeV/u energy loss is dominated by electronic collisions. These collisions are statistical processes and because the number of interactions of a given projectile is in general large, for studying its stopping, an average energy loss is defined [13]. Electronic stopping power of heavy charged particles in matter is described by the semiclassical Bethe-Bloch formula [15, 16, 17]:

\[
\frac{dE}{dx} = \frac{4\pi e^4 Z_t^2}{m_e c^2 \beta^3} \left[ \ln \frac{2m_e c^2 \beta^2}{\langle I \rangle (1 - \beta^2)} - \beta^2 \right] + \text{corrections},
\]

where \( m_e \) is the rest mass of the electron, \( \beta = V/c \), \( V \) the velocity of projectile, \( c \) the speed of light in vacuum, \( Z_p \) the atomic number of the projectile, \( Z_t \) the atomic number of the target and \( \langle I \rangle \) the mean ionization potential of the target material, a constant which describes in some sense the ability of the target to absorb energy from the incident projectile.

In spite of the enormous amount of work devoted to stopping powers and ion ranges, it is still not possible to calculate accurately ion stopping power truly from first principles. Phenomenological parameters such as \( \langle I \rangle \)-value are required to pin the calculations to data. The mean ionization potential can be defined as the first energy moment of the dipole oscillator strength distribution and it can be evaluated theoretically by using a quantum model, but the choice of a particular wave function may have an unacceptably large effect on the retrieved values [18, 19]. On the other hand, oscillator strength measured values were also taken into the definition to retrieve \( \langle I \rangle \)-values for complex molecules [20, 21, 22]. The mean ionization potential can be obtained alternately by fitting experimental stopping data to a physical model but in this case the retrieved values will contain higher-order Born contributions to the stopping power and energy loss mechanisms which are usually neglected in the models [19, 23].

As mentioned previously in literature, determination of the mean ionization potential is the principal non-trivial task in the evaluation of the Bethe stopping power formula [24, 25, 26]. Recommended values have varied substantially in...
time. Estimates of $<I>$ based on experimental stopping power measurements of protons, deuterons, and alpha particles were given in ICRU37 [27] and retained in ICRU49 [28]. The newly evaluated $<I>$-values based on oscillator-strength distributions and dielectric-response functions for chemical elements were given in ICRU73 [29]. In a previous work [26] the effects of the $<I>$-value uncertainty on the Bragg position solely were reported for 290 MeV/u $^{12}$C ions in water.

Liquid water as a stopping medium for energetic heavy ions plays a major role in medical applications of ion beams. It is the most common type of material used for phantoms of human body and many of the current treatment planning systems use water-equivalents of human tissues. The recommended $<I>$-value for water in ICRU37 and ICRU49 is $(75 \pm 3)$ eV. A much lower value of 67.2 eV is calculated in ICRU73. The $<I>$-values reported by different authors cover quite a large range: 77 eV [30] from fitting experimental data to a Monte Carlo based treatment planning system, 77.8 eV [22] by using a dielectric response stopping model for liquid water, $(79.7 \pm 2)$ eV [31] from 70 MeV proton stopping data, 81.8 eV [32] by using electron inelastic-scattering cross sections, $(80.8 \pm 2)$ eV [33] from comparison of experimental ranges to results of various stopping codes, $(80\div85)$ eV [34] by using optical loss functions, etc.

In the present study we attempt to assess values for the mean ionization potential $<I>$ by comparing available experimental Bragg data for carbon ion beams in water with Monte Carlo (MC) simulations in a new approach involving a set of three shape parameters the Bragg curve. To cover the entire range of $<I>$-values reported in literature, for the present study we selected the values: 67.2, 75, 78, 80, 82, 83 and 85 eV. Our comparison involves the Bragg peak position (BPP) in the same way other studies do – e.g. [30, 35, 36] and, for the first time, three more parameters which describe the shape of the Bragg peak are added to the comparative study: the full width at 3/4-th of the maximum value (denoted by FW3/4M), the full width at half maximum (FW1/2M) and the full width at 1/4-th of the maximum value (FW1/4M). All measured Bragg curves at incident beam energies in the therapeutic range were considered in the present study (to the best of our knowledge). The simulations were performed with the well known Monte Carlo transport codes FLUKA and PHITS.

3. EXPERIMENTAL DATA AND THE PROCEDURE EMPLOYED FOR ERROR ESTIMATES

The interaction between carbon ion beams of energies suitable for hadrontherapy (100÷400 MeV/u) and water as a tissue-like medium was experimentally investigated in extenso. Most of the measurements were performed at GSI Darmstadt and RIKEN Japan. The data employed in the present study for comparison with the simulation results are from [30, 37, 38, 39].
For carbon ion beams in water with energies from 100 to 400 MeV/u in steps of 50 MeV/u, results of measurements at GSI in 2007 were used. Bragg curves of carbon beams normalized to the entrance point are reported by Steidl [39]. Although the curves at 100 MeV/u and 400 MeV/u were not completely measured in the entrance plateau and tail region, due to minimum and maximum limits of the range telescope, the core data contained all the necessary information on the shape parameters of the corresponding Bragg curves, required by the present investigation.

Data concerning 135 MeV/u $^{12}$C ions in water were originally measured at RIKEN [40] however in the present study we used as a source reference O. Geithner's Dissertation [38]. The same work was used to retrieve experimental data at 195, 270 and 330 MeV/u. These Bragg curves data were originally measured at GSI and reported in [37]. Similarly, depth dose profile experimental data for 390 MeV/u $^{12}$C ions in water were measured at GSI and were obtained from [41].

In the absence of a reported numerical value, the experimental error interval in position was taken to be of the order of the linear dimension for each symbol used to represent a data point. The BPP, FW3/4M, FW1/2M, FW1/4M values and the associated estimates of errors were extracted from the previously mentioned references. All geometrical values were expressed in mm.

BPP was determined as the depth coordinate of the highest energy deposition data point. For some incident energies this is an approximation and a more accurate value could be obtained by fitting the experimental data lying in the Bragg peak region to a Gaussian, a procedure beyond the purpose of the present work.

The experimental value of each shape parameter was determined as a difference between the abscissas of two points lying on each side of the Bragg peak centroid, whose corresponding ordinates are 3/4, 1/2 and 1/4 respectively of the maximum height. The pairs of points were considered on the linearly interpolated experimental curve. By connecting those points, three horizontal lines at each fraction of the maximum height were obtained. In each case, an estimate of the error interval was evaluated. The minimum and maximum values of this interval correspond to the difference between the abscissas of the closest (in the ordinate direction) experimental data points located above (minimum) and below (maximum) the horizontal direction that was used to measure each shape parameter.

In Figs. 1 to 3 the experimental Bragg curves of $^{12}$C stopped in water for the twelve incident energies considered in this work are represented together with the corresponding FLUKA and PHITS calculations. For consistency, the simulation results were normalized in the entrance plateau to the experimental data. The calculated values are obtained for a mean ionization potential $<I> = 80$ eV. The length scale in the incident beam direction was chosen differently for incident beam energies belonging to three ranges: 100 ÷ 195 MeV/u, 200 ÷ 300 MeV/u and 330 ÷ 400 MeV/u, in order to allow comparison of experimental data and simulated results without loss of details. The same scaling procedure was applied in the energy deposition axis.
In Figs. 4 to 15, panels of graphs containing experimental and calculated parameter values are presented. In each graph, the corresponding experimental value of BPP (a), FW3/4M (b), FW1/2M (c), and FW1/4M (d), respectively, is shown as a horizontal continuous line extending over the selected range of \(<I>\)-values. Similarly, the minimum and maximum values determined by the estimated experimental uncertainties are represented as dashed lines, defining on each graph a shaded area representative of the estimated error interval.

The scale in the ordinate direction covered the same distance interval at all energies, namely: 10 mm in BPP, 5 mm in FW3/4M, 15 mm in FW1/2M and 120 mm in FW1/4M, in order to allow for direct comparison. The maximum value which was chosen in the FW1/4M representation is quite large, because it needs to accommodate the large deviations of the simulated data from the experimental ones and among each other for this particular shape parameter. Also, at the highest incident beam energies of 390 and 400 MeV/u the FW1/4M could not be estimated because that level was below the entrance plateau both in the measured and in the simulated Bragg curves.

4. CALCULATIONS

The simulations were carried out using the FLUKA code Version [2008. 3b. 2] [11] and the Particle and Heavy-Ion Transport code System PHITS – Version 2.08 [12]. Both simulations considered the same type of source i.e. a monoenergetic axial pencil beam of carbon ions, the same target geometry and composition. The incident energy values coincide with those previously used in the measurements of the Bragg curve data.

The target was modeled as a cylindrical water volume with the symmetry axis in the direction of propagation of the incident beam, surrounded by air. The length of the water target was 40 cm, longer than the range of the most energetic projectiles employed in the simulations and the radius was 10 cm, of the order magnitude of the human body transverse dimension. The air region surrounding the water target was 50 cm length and 20 cm radius in this simplified model. The total energy deposition was scored in 0.1 mm width bins in the direction of the incident beam.

FLUKA code performs the transport of therapeutic \(^{12}\text{C}\) ion beams by using an original multiple Coulomb scattering algorithm [42] based on Moliere multiple scattering theory [43, 44]. The ionization energy loss is computed by Bethe-Bloch theory in a statistical approach [45]. Nucleus-nucleus interactions are supported by interfacing with DPMJET-III [46] and with a modified version of RQMD-2.4 implementation [47, 48]. Evaporation and fission of the excited residual nuclei are described by a new version of the Weisskopf theory [49]. FLUKA was run using the defaults of HADRONThERAPY option which includes Electromagnetic
FLUKA (EMF) and inelastic form factor corrections to Compton scattering, particle transport threshold at 100 keV, delta ray production with a threshold at 100 keV.

Based on NMTC/JAM code [50], PHITS uses NASA systematic [51] for computing the total reaction cross sections of heavy ions and subsequently the mean free path of the transport carbon ion which determines the selection of the next collision point by MC method. The default option for computing the ionization energy loss is the Spar code [52] but in the present simulations the recently implemented ATIMA [53] code option was used. Only in this case PHITS provides a parameter allowing for arbitrary input \( <I> \)-value. The code was run with an option to calculate ionization energy loss by ATIMA for nucleus and proton and by NMTC/JAM for any other particle, with Coulomb diffusion and energy straggling. The minimum energy for range calculation of charged particles was 1 eV, the proton cut-off energy was \( 10^{-3} \) MeV, the neutron cut-off energy was 1 MeV and the cut-off energy for all the other particles, including heavy ions was \( 10^{-6} \) MeV. The fragmentation of the incident projectiles and other nucleus-nucleus reactions are taken into account as a two-step process whose modeling involves the JQMD model [50] for the dynamical stage and GEM model [54] for the light particles evaporation and fission of the excited residual nuclei stage. With the exceptions mentioned before, all the other model options used in the present simulations were the default ones.

5. RESULTS AND DISCUSSIONS

As mentioned in Section 2, the mean ionization potential is an important parameter entering the calculations of the electronic stopping power (Eq. (2)). Usually \( <I> \) is derived by adjusting its values in a physical range in order to obtain best description of BPP. This approach was adopted for example in the studies reported in [29, 30, 35]. In the present study we extended this approach in two ways: (i) by considering the Bragg peak shape parameters (BPSP) simultaneously with the BPP to decide upon the best fit simulation results; (ii) by comparing the calculations with a large set of experimental data.

A possible way to achieve an agreement between the particle range predicted by FLUKA and PHITS with the measured one is to adjust \( <I> \) of the stopping medium to an optimum value. The FLUKA and PHITS default \( <I> \)-value is set to 75 eV, according to ICRU49 recommendations (75 ± 3) eV. Recent effectively calculated \( <I> \)-value for water is 67.2 eV. Different \( <I> \)-values for water, up to 85 eV can be found elsewhere [34]. Therefore in the present study we investigated the sensitivity of the BPP and BPSP on the \( <I> \) parameter and made comparison with available experimental data at these \( <I> \)-values lying between 67.2 and 85 eV.
The experimental depth-dose curves of $^{12}$C ions in water at incident energies in the $100\div195$ MeV/u range are illustrated in Fig. 1. The shape of the distributions is well reproduced, while the peak position is underestimated in calculations by 1.2 mm at 100 MeV/u, 0.5 mm at 135 MeV/u, 1.5 mm at 150 MeV/u and 1.0 mm at 195 MeV/u. FLUKA and PHITS calculations are consistent with each other. Simulated curves correspond to $<I>_0 = 80$ eV. As shown in Fig. 2, the experimental BPP for $^{12}$C ions in water is satisfactorily described by calculations at 270 MeV/u, but a certain underestimation appears at 200, 250 and 300 MeV/u. The $<I>_0$-value used in this case was also $<I>_0 = 80$ eV.

The experimental Bragg curves in the $330\div400$ MeV/u range are shown in Fig. 3 in comparison with calculations. Simulation results by FLUKA and PHITS using the optimal value of ionization potential ($<I>_0 = 80$ eV), were found to agree well with experimental data in the entrance region and in the position of the Bragg peak. This supports the reliability of the FLUKA and PHITS electromagnetic models after the adjustment of the mean ionization potential. From Fig. 3 it can be observed that the dose beyond the Bragg peak (tail) predicted by FLUKA is in agreement with the experimental data, indicating a good account of the nuclear processes (fragmentation).

The analysis of BPP and BPSP at incident energy of 100 MeV/u is depicted in Fig. 4. The agreement between FLUKA and PHITS simulations on BPP is good while comparison of both of them with the experimental data gives 8.3% relative change at $<I>_0 = 67.2$ eV and 4.4% for the other $<I>_0$-values. Calculated BPP values (Fig. 4a) get into the uncertainty interval (shaded area) at $<I>_0$-values larger than 75 eV. Therefore this parameter alone cannot discriminate a certain $<I>_0$-value in the $75\div85$ eV range. But comparison of experimental with simulations for the BPSP (panels (b), (c), and (d)) shows clearly that $<I>_0$-values in the $78\div82$ eV range give the best description of the experimental points. At 100 MeV/u, BPSP analysis provides unambiguously the optimum range of values for $<I>_0$. The resulting data for FW3/4M, FW1/2M and FW1/4M presented in Fig. 4 show that a better agreement with experimental data is obtained at $<I>_0 = 80$ eV for both codes.

The calculated BPP and BPSP values in comparison with experiment at 135 MeV/u are presented in Fig. 5. The difference between the results of FLUKA and PHITS simulations on the BPP is near zero except at $<I>_0 = 85$ eV, where 2.3% relative change can be observed between the two simulations. Comparison of both calculations with experimental data shows 3.4% relative change at $<I>_0 = 67.2$ eV and 1.1% for $<I>_0$-value in the $75\div83$ eV range. BPP values (Fig. 5a) enter the uncertainty interval (shaded area) at $<I>_0$-values larger than 75 eV. Therefore, based only on this parameter, a definite $<I>_0$-value for water cannot be selected. The comparison of calculations with experimental data for BPSP (Fig. 5b, c and d) indicate the best agreement at $<I>_0 = 78$ eV.
Fig. 1 – Expanded part of the experimental Bragg curves of $^{12}$C ions in water at incident energies of 100, 135, 150 and 195 MeV/u (open symbols). FLUKA and PHITS results at $\langle \tilde{l} \rangle = 80$ eV are represented by continuous and dotted lines, respectively. See text for details and comments.

Fig. 2 – Similar to Fig. 1 for incident energies of 200, 250, 270 and 300 MeV/u.
Fig. 3 – Similar to Fig. 1 for incident energies of 330, 350, 390 and 400 MeV/u.

Fig. 4 – Bragg peak position (panel (a)) and Bragg peak shape parameters (panels (b), (c), (d)) for $^{12}$C ion beams in water at incident energy of 100 MeV/u. Experimental values (horizontal continuous line) and their corresponding uncertainty interval (shaded area) are compared to calculations performed by FLUKA (open symbols) and PHITS (dark symbols). The selected $\langle I \rangle$-values are those reported in the literature.

Dotted lines connecting the symbols are for guiding the eye. See text for details and comments.
The simulated BPP and BPSP values at 150 MeV/u incident beam energy are plotted against experimental data in Fig. 6. FLUKA and PHITS give similar results concerning BPP except at $<I> = 85$ eV, where a 1.9% relative change can be observed. Comparison of both calculations with experimental data indicates a 4.6% difference at $<I> = 67.2$ eV and 2.7% at $<I>$-values in the 75–85 eV range. At $<I> = 85$ eV PHITS shows 0.8% relative change to experimental data while FLUKA gives 2.7% difference. In Fig. 6 the calculated BPP values are close to the uncertainty interval (shaded area) for all $<I>$-values larger than 75 eV, therefore this parameter alone cannot be used to select a narrower $<I>$-value range. Comparison of experiment with simulations for the BPSP (panels (b), (c), and (d)) shows clearly that $<I>$-values in the 78–80 eV range give a better reproduction of the experimental data points. The value $<I> = 67.2$ eV produces simulation results which are in good agreement with experimental data in the BPSP analysis, but it is ruled out by a larger imprecision of the BPP prediction (4.6% relative difference with respect to experimental data for both codes, as compared to 2.7% in the other cases). In conclusion, at 150 MeV/u incident energy the combined BPP and BPSP analysis provides a narrow range of values for $<I>$: 78–80 eV.

As shown in Fig. 7, the BPP calculated with FLUKA and PHITS at 195 MeV/u provide a description of experimental data with a precision better than 3 mm. The
difference between the two calculations at this energy is negligible for all \(<I>\)-values considered in this work. A noticeable discrepancy (up to 3.6%) is observed between simulation results and experimental data if \(<I>\) ranges in the 67.2÷78 eV interval, as can be seen in Fig. 7a. By increasing the \(<I>\)-value of water in the 80÷85 eV range, BPP values get into the uncertainty interval and both calculations provide descriptions of experimental results within 1.2% precision. Based only on the BPP values, a narrower range of \(<I>\)-values cannot be selected. On the other hand, the comparison experiment-calculation for the BPSP values presented in Fig. 7b,c,d) shows up clearly that \(<I>\)-values lying in the very restrictive range 82÷83 eV are in good agreement with experimental data, while keeping the best description of the measured BPP. The ICRU73 value \(<I>\>=67.2\) eV gives again comparatively good simulation results concerning BPSP values but it is ruled out by the large difference of predicted BPP relative to the experimental value.

Fig. 6 – Similar to Fig. 4 at incident energy of 150 MeV/u.
Fig. 7 – Similar to Fig. 4 at incident energy of 195 MeV/u.

Fig. 8 presents simulation results of the two codes against experimental data concerning $^{12}$C ion beams at 200 MeV/u. For the BPP a 1.2% difference between FLUKA and PHITS results was obtained at $\langle I \rangle = 82$ eV. The other considered $\langle I \rangle$-values produced the same BPP values by both codes (Fig. 8a). A comparison between simulations and experiment shows that the predicted BPP values are 3.9% apart from experiment at $\langle I \rangle = 67.2$ eV and 1.6% apart for $\langle I \rangle$-value in the $75\div80$ eV range. The relative change between the calculated and experimental BPP values for $\langle I \rangle$ in the $83\div85$ eV range is 0.5%. A comparison of the simulated and measured BPSP (Fig. 8b,c and d) indicates that $\langle I \rangle$-values of 78 eV and in the $83\div85$ eV range provide the best agreement between simulation and experiment. In conclusion, the BPSP analysis at this incident energy confirms the $\langle I \rangle$-values retrieved by BPP fit.
Fig. 8 – Similar to Fig. 4 at incident energy of 200 MeV/u.

Data on BPP and BPSP in 250 MeV/u incident energy are illustrated in Fig. 9. In Fig. 9a it can be observed that the relative difference between FLUKA and PHITS calculations is 0.8% at the $<I>$-values equal to 75, 80 and 85 eV, while the other $<I>$-values yield similar results by both codes. Comparison of the BPP calculations with experimental data shows a 0.2% relative change to the experimental data for $<I>$ ranging in the 82÷83 eV interval. Unlike PHITS, FLUKA produces the same small relative change at $<I>=80$ eV. Data on BPSP (Fig. 9b, c, d) illustrate good agreement between simulation results and experiment for $<I>=78$ eV and for values in the 82÷83 eV range. At these values of $<I>$, FLUKA predicted results are closer to the experimental data than PHITS, which is probably related to the nucleus-nucleus interaction model in use. In conclusion, BPSP analysis narrows down to 82÷83 eV the wider ranges 80÷85 eV, obtained from BPP fit.
The calculations of BPP and BPSP in comparison with experiment are illustrated in Fig. 10 for the incident beam energy of 270 MeV/u. The relative difference between the predictions of FLUKA and PHITS simulation codes on the indicator BPP is negligible except at the $<I>$ = 78 and 82 eV, where a 0.7% relative difference can be observed. Comparison of both calculations with experimental data gives a 2.4% relative difference at $<I>$=67.2 eV and 1.1% at $<I>$ = 75 eV. At 78 eV FLUKA results provide a 0.4% difference with respect to the experiment, while PHITS predicted BPP values present 1.1% difference. For $<I>$-values in the 80÷85 eV range both codes predict BPP values which are well near the experimental data (0.4–0.3% difference), thus making difficult the selection of a more restrictive range for the appropriate $<I>$-value. Comparison of experimental to simulations for the BPSP values (Fig. 10b, c, d) shows that $<I>$ = 80 eV is a good choice for the mean ionization potential which takes the simulated BPSP values close to the experimental (even 0.5% difference in FW1/2M for FLUKA). At this incident energy, a reasonable agreement between simulation results and experimental data for all considered observables occur for $<I>$-values in the 83÷85 eV range and at 80 eV.
Figure 11 shows the BPP and BPSP values of $^{12}\text{C}$ ion beams incident at 300 MeV/u. The values of BPP at $<I> = 75$ eV as default $<I>$-value of FLUKA and PHITS gives 1% and 1.6% difference to experimental data, respectively. At higher $<I>$-value, the relative difference between simulations and experiment in the BPP value decreases and reaches −0.2%. Data predicted on the BPSP by FLUKA and PHITS display a different evolution relative to the experimental values and, overall, if $<I>$ range in the 80÷82 eV interval, the best agreement is achieved. By inspecting Fig. 11c, d the conclusion can be drawn that the corresponding BPSP values predicted by FLUKA calculations are close to the experimental data, within the 80÷82 eV range and especially at $<I> = 80$ eV. The observables considered in these panels are expected to be more sensitive to the nuclear interaction model. Therefore, as observed before, it can be concluded that a more appropriate nuclear model is used as default option in the FLUKA code.
The experimental and calculated BPP and BPSP values corresponding to 330 MeV/u incident energy are plotted in Fig. 12. At this energy, the FLUKA and PHITS results still underestimate the BPP experimental data for mean ionization potential values smaller than 80 eV. \( \langle I \rangle \)-values in the 80÷85 eV range take the simulation results on BPP into the uncertainty (shaded) area. The best reproduction of experiment is obtained at \( \langle I \rangle = 85 \) eV by FLUKA calculations. Comparison of the calculated BPSP with experimental data indicates a different behavior of the simulation results by FLUKA and PHITS, as shown in Fig. 12d. Based on the BPSP data, it can be observed that the best agreement between simulation results of both codes and experiment is obtained when \( \langle I \rangle \) is within the 80÷82 eV interval, while the BPP indicator shows the best agreement with the experimental data in the wider 80÷85 range. Fig. 12d shows that FLUKA calculations are closer to the experiment.
Figure 13 presents simulation results and experimental data on BPP and BPSP at 350 MeV/u incident energy. The calculated BPP values shown in panel (a) are in the uncertainty interval (shaded area) for \(<I>\)-values lying in the 78÷85 eV range. The behavior of the simulation results on BPSP obtained by the two codes is quite different: while PHITS clearly overestimates the BPSP, FLUKA reproduces the experimental data to a much better extent, especially for \(<I>\)-values in the 80÷85 eV range, as can be seen in Fig. 13b, c, d. The simulation results obtained by FLUKA illustrate a smooth behavior of the calculated BPSP points which are closer to experiment than the PHITS values. In the favorable range of \(<I>\)-values, the difference between FLUKA calculated BPSP and experimental data does not exceed 10% (with one exception, FW1/2M at 82 eV) while the PHITS simulated BPSP values are affected by relative differences to experiment which can amount to almost 50%. In spite of these differences, it can be observed that the most favorable range for the \(<I>\)-value is consistently predicted by PHITS and FLUKA, \textit{i.e.} 80 ÷ 85 eV, thus proving that BPSP analysis is useful even when the description of the absolute values of the experimental data is less accurate.
The behavior of the calculated BPP and BPSP observables at 390 MeV/u, incident energy relative to the experimental values is presented in Fig. 14a where one illustrates an almost linear correlation between BPP and $<I>$-value. For $<I>$ in the 75÷85 eV interval a very good agreement between the simulated BPP and the experimental data is obtained, corresponding to less than 1% difference. Comparison of experimental data with simulation results for FW3/4M (Fig. 13b) shows that the best agreement with experimental data is achieved in the 80÷82 eV range. Relative differences between PHITS simulated BPSP values and experimental FW3/4M values is less than 13% while for FLUKA results the corresponding error is less than 40%. Fig. 14c indicates that FW1/2M experimental values are better described by PHITS.
Fig. 14 – Similar to Fig. 4 at incident energy of 390 MeV/u. Note that FW1/4M cannot be determined at this energy, as discussed in Section 3.

At 400 MeV/u incident energy of $^{12}$C ion beam, the calculated BPP and BPSP values are shown in Fig. 15 against the experimental data. Fig. 15a exhibits a quasi-linear correlation between BPP and $\langle I \rangle$-values. In the $78\div85$ eV range the simulation results get into the experimental uncertainty area (the relative differences are less than 1%). For $\langle I \rangle$ ranging in the $82\div85$ eV interval a positive relative difference between simulation results and experimental data can be observed, and in the $78\div80$ eV interval calculations underestimate the experiment. The FW3/4M calculated values are lying in the uncertainty area throughout the entire range of $\langle I \rangle$-values. Slightly better results are given by FLUKA simulations for the $\langle I \rangle$-values in the $75\div85$ eV interval. As far as the FW1/2M indicator is concerned, FLUKA calculations are closer to the experimental values. At this incident energy, a confirmation of the $\langle I \rangle$-values retrieved by BPP fit analysis is obtained by considering the BPSP indicators.
6. CONCLUSIONS

In the present work the Bragg peak position (BPP) and Bragg peak shape parameters (BPSP) of $^{12}$C ions stopped in water targets were employed in order to obtain better empirical estimates of the mean ionization potential $\langle I \rangle$ of water. A comprising set of published experimental data for $^{12}$C ion beams at incident energies relevant for hadrontherapy: 100, 135, 150, 195, 200, 250, 270, 300, 350, 390 and 400 MeV/u were considered in order to compare with the numerical simulations performed by the PHITS and FLUKA computer codes. A careful scanning of the literature revealed $\langle I \rangle$-values for water ranging from 67.2 to 85 eV. The calculations reported in this paper make use of $\langle I \rangle$-values in this range, including all figures proposed in previous studies.

Comparisons of the simulation results with experimental data are shown in Figs. 4–15. In Fig. 16, a comparative representation of the most favorable $\langle I \rangle$-values obtained by the BPP fit method and by imposing experimental constraints to all BPSP observables are presented. This figure indicates unambiguously that at all incident energies a narrower range of favorable $\langle I \rangle$-values is obtained if BPSP
observables are considered along with the BPP one. This conclusion stands out most clearly at the lowest incident energies considered here, namely 100, 135, 150, 195, 250, and 270 MeV/u, where the Bragg curves are less perturbed by the nuclear processes. An exception is the 200 MeV/u incident energy, where the range of the $<I>$-values determined by the BPP fit analysis is already quite narrow - 83÷85 eV and it is confirmed by the combined method.

At all incident energies FLUKA and PHITS predictions concerning the BPP are very close to each other (Figs. 4 to 15, panel a). On the contrary, for the BPSP indicators, the results retrieved by the two codes are sometimes different, especially at higher energies, where the nuclear contribution is expected to increase. The FW3/4M shape parameter is less sensitive to the nuclear interactions. Indeed, by inspecting the panel b of Figs. 4–15, the results of both codes are similar. A slightly better reproduction of experiment for this indicator is provided by PHITS at 330 and 390 MeV/u incident energies. The FW1/2M shape indicator (panel c) retrieved by FLUKA and PHITS has almost identical values at 100, 135, 150 and 195 MeV/u. At higher energies FLUKA predictions are better, except at 330 MeV/u (Fig. 12c). For all incident energies considered in the present study the FW1/4M shape indicator (panel d of Figs. 4–12) is better described by FLUKA. This can be observed very clearly at energies above 250 MeV/u (Figs. 9–12, panel d) thus indicating a proper selection of the nuclear model in the default option of FLUKA.

Fig. 16 – A comparative representation of $<I>$-values obtained from BPP fit analysis (open bars) and those obtained by imposing experimental constraints on all observables of BPSP analysis (shaded bars).
As seen in Fig. 16, at 10 out of the 12 incident energies investigated in the present study a narrower range of $<I>$-values has been obtained as a result of the BPSP analysis, comparatively with the values retrieved by the BPP fit analysis. For the other two energies (200 MeV/u and 400 MeV/u) the analysis based on the shape parameters confirms the favorable $<I>$ range obtained by using BPP fit analysis.

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REFERENCES

38. O. Geitbner, Monte Carlo simulations for heavy ion dosimetry, Dissertation, Heidelberg University, 2006.


