Analytical expressions for water-to-air stopping-power ratios relevant for accurate dosimetry in particle therapy

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Abstract

In particle therapy, knowledge of the stopping-power ratio (STPR) of the ion beam for water and air is necessary for accurate ionization chamber dosimetry. Earlier work has investigated the STPR for pristine carbon ion beams, but here we expand the calculations to a range of ions ($1 \leq z \leq 18$) as well as spread-out Bragg peaks (SOBPs) and provide a theoretical in-depth study with a special focus on the parameter regime relevant for particle therapy. The Monte Carlo transport code SHIELD-HIT is used to calculate complete particle-fluence spectra which are required for determining the STPR according to the recommendations of the International Atomic Energy Agency. The STPR at a depth $d$ depends primarily on the average energy of the primary ions at $d$ rather than on their charge $z$ or absolute position in the medium. However, STPRs for different sets of stopping-power data for water and air recommended by the International Commission on Radiation Units and Measurements are compared, including also the recently revised data for water, yielding deviations up to 2\% in the plateau region. In comparison, the influence of the secondary particle spectra on the STPR is about two orders of magnitude smaller in the whole region up till the practical range. The gained insights enable us to propose simple analytical expressions for the STPR for both pristine and SOBPs as a function of penetration depth depending parametrically on the practical range.

(Some figures in this article are in colour only in the electronic version)
1. Introduction

Stopping powers are essential for calculating the dose deposited by ionizing particles. The deposited dose is described as the mass stopping power multiplied with the particle fluence, while assuming charged particle equilibrium from the short-ranged delta electrons. At particle-therapy centers, air-filled ionization chambers are routinely used as a main tool for quality assurance of the delivered beam. Several dosimetry protocols for protons have been conceived while the most recent protocol provided by the International Atomic Energy Agency (IAEA) TRS-398 (IAEA 2000) sets the standard in proton dosimetry today. In addition, TRS-398 also covers dosimetry for ions heavier than protons. The protocol uses an absorbed dose-to-water-based formalism and relates the dose to water $D_{\text{w}, Q}$ to the acquired charge $M_Q$ multiplied by a calibration factor $N_{D, \text{w}, Q_0}$ and a dimensionless beam quality correction factor $k_{Q, Q_0}$. The correction factor $k_{Q, Q_0}$ relates the measured beam quality $Q$ to the beam quality $Q_0$ used for calibration of the dosimeter and it is defined in TRS-398 as

$$ k_{Q, Q_0} = \frac{(S_{\text{water/air}})_Q}{(S_{\text{water/air}})_{Q_0}} \cdot \frac{(W_{\text{air}})_Q}{(W_{\text{air}})_{Q_0}} \frac{p_Q}{p_{Q_0}} \quad (1) $$

including the water-to-air stopping-power ratio $S_{\text{water/air}}$, the mean energy expended in air per ion pair formed $W_{\text{air}}$, and a perturbation factor $p_Q/p_{Q_0}$, which considers effects for the specific ionization chamber used. While there is an on-going trend to experimentally determine the chamber- and beam-specific $k_{Q, Q_0}$ factors, this effort is far from being completed. Until this is achieved, there is a need to rely on calculated $k_{Q, Q_0}$ factors tabulated in dosimetry recommendations.

As mentioned in TRS-398, calculating the correct beam quality factor in particle therapy is complex since it involves knowledge of the entire particle-energy spectrum at the point of interest. Instead, TRS-398 proposes a pragmatic approach by recommending a fixed value of 1.13 as a generic correction factor for the dosimetry of ions heavier than protons based on the analysis by Hartmann et al (1999), irrespective of the particle types and energy spectra which are functions of depth. Accordingly, TRS-398 summarizes that the estimated combined standard uncertainty in $k_{Q, Q_0}$ in ion beams heavier than protons (about 3%) arises largely from the uncertainty of the stopping-power ratio (STPR) (about 2%) and the value for $W_{\text{air}}$ (about 1.5%). This has been taken up by Henkner et al (2009), Paul et al (2007) and Geithner et al (2006) for mono energetic carbon beams, and they found out that (i) the STPR is not constant but varies with penetration depth, and (ii) it depends strongly on the accuracy of the stopping-power data used as an input for the calculation. Accordingly, it was concluded that in a clinical setting an over or under dosage may occur in the order of a few percent.

Here, we shall continue the initiated work on STPRs focusing on two objectives: first, gaining a sound understanding of the physics determining the STPR, and second, exploiting the gained understanding in order to provide results with direct clinical relevance which are ready to be applied in clinical practice in a quality assurance setting.

The deeper insight in the context of the STPR is required since the STPR strongly depends on the stopping-power data which are used for its determination. The problem is, however, that the stopping-power data currently recommended by the International Commission on Radiation Units and Measurements (ICRU) possess some intrinsic inconsistencies. In contrast to an accurate but purely numerical calculation of STPRs, a sound understanding of the relevant physics allows for conclusions independent of the employed set of stopping-power data. It is also a prerequisite for an analytical description of the STPR. In this context it

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6 Although the study of the value for $W_{\text{air}}$ is beyond the scope of this work, it shall be mentioned that the estimated uncertainty for $W_{\text{air}}$ calls for a detailed investigation.
Analytical expressions for water-to-air stopping-power ratios may be mentioned that a close relation exists between the calculation of STPRs and water equivalent ratios which are studied, for example, in Zhang and Newhauser (2009). It should be emphasized that, in contrast to earlier work on the STPR (Henkner et al. 2009, Geithner et al. 2006, Paul et al. 2007), this study also considers the recently revised ICRU 73 (ICRU 2005) stopping-power data for ions heavier than helium on water. These data replace the ones originally published in ICRU 73 which led to a still ongoing discussion on stopping powers for water targets (see, e.g., Paul (2010)) especially in view of recent measurements by Schardt et al. (2008). Obviously, there are several other sources of stopping-power data readily available such as SRIM (Ziegler 2010) and ATIMA (Geissel et al. 2011) to name only two. While ATIMA is used with advantage at very high energies, being based on the fully relativistic theory by Lindhard and Sørensen (1996), SRIM, based on the work by Ziegler (1977), works in general fairly well for all ions and for all energies with some exceptions at lower energies (Paul 2010). Furthermore, SRIM is electronically available and therefore frequently used for applied calculations also including particle therapy. However, the objective of this study is to improve the general understanding of the STPR and a comparison of the large body of stopping-power data is beyond its scope.

TRS-398 explicitly states that the STPR for water-to-air, $S_{\text{water}/\text{air}}$, should be obtained by averaging over the complete spectra of particles present. And consequently, this requirement was considered to be an important limitation in the case of heavy charged particles, where the determination of all possible particle spectra was assumed to be a considerable undertaking. This was certainly the case a decade ago and may still be true from the point of view of dose determination for routinely quality assurance. Nowadays, however, the determination of the complete spectra of particles can be achieved conveniently and with high accuracy by applying Monte Carlo transportation codes exploiting the commonly available computer power. These codes are in general valuable in predicting radiation fields of ions in tissues and are in particular useful in hadron therapy for the simulation of ion transport. The most common codes in particle therapy with ions heavier than protons are Geant4 (Agostinelli et al. 2003), FLUKA (Fassò et al. 2005), PHITS (Iwase et al. 2002), MCNPX (Pelowitz 2005), and SHIELD-HIT (Dementyev and Sobolevsky 1999, Gudowska et al. 2004), all taking into account the atomic interaction of the ions with the target medium as well as the nuclear interaction. It is the former interaction which mainly determines the energy loss of the incident ions and therefore the stopping power, while the latter interaction is responsible for fragmentation and therefore for the production of secondary-particle spectra.

Initial studies on STPRs relevant for dosimetry in radiation therapy with ions heavier than protons were performed without Monte Carlo calculations ignoring the influence of the secondary particle spectrum (e.g. Salamon (1980), Hiraoka and Bichsel (1995), ICRU (1993) as presented in TRS-398 (IAEA 2000)). Calculations exploiting the capabilities of Monte Carlo codes were performed with SHIELD-HIT but exclusively carbon-ion fields (Geithner et al. 2006, Paul et al. 2007, Henkner et al. 2009) were studied. However, the dependence of the STPR on different ion species is of interest since a number of facilities world-wide (e.g., NIRS and HIT) are equipped with radiation fields which cover a broader range of ions than merely protons and carbon ions. Furthermore, it was recently argued that ions heavier than carbon may play an important role in the near future concerning the radiation therapy of radio-resistant tumors (Bassler et al. 2010a). Consequently, a large variety of ion species, namely H, He, Li, C, N, O, Ne, Si, and Ar, are considered here—all accessible either for clinical radiation therapy (up till O and Ne at HIT and NIRS, respectively) or for in vitro radiobiology experiments.

Despite their obvious relevance in medical application, so far, STPRs for spread-out Bragg peaks (SOBPs) for ions heavier than protons have been discussed only scarcely in the
Table 1. Specifications of four SOBPs for carbon ions in water. Given are the width along the beam axis, the practical range $R_p$, and the optimization of the SOBP for a homogeneous physical dose or relative biological dose. The optimization was performed by the treatment planning program TRiP (Krämer et al 2000, Krämer and Scholz 2000).

| SOBP | Width (mm) | $R_p$ (mm) | Optimization |
|------|------------|------------|--------------|
| a    | 50         | 220        | Physical     |
| b    | 80         | 168        | Physical     |
| c    | 50         | 150        | Physical     |
| d    | 100        | 153        | Biological   |

literature, namely by Henkner et al (2009). In the case of proton beams, more detailed efforts have been performed, e.g., by Palmons and Verhaegen (1998) and Palmons and Vynckier (2002), and earlier already by Medin and Andreo (1992). Henkner et al, who considered carbon ions, outlined in the conclusions of Henkner et al (2009) that a more detailed analysis of STPRs for SOBPs is clearly needed since their statements were only based on the analysis of a single physically optimized SOBP using one set of stopping-power data. Consequently, one focus of this work should be a systematic study of the STPR for SOBPs, both physically and biologically optimized, of different widths and practical ranges leading to an analytic expression for the STPR.

This paper is organized as follows: first, the physics relevant for the STPR and the employed methods are discussed. Furthermore, analytical expressions for the average energy of the primary ions and STPRs are proposed. Subsequently, the results for the water-to-air STPR for pristine as well as SOBPs are presented and compared to the proposed analytical expressions. The following discussion concentrates on three issues, namely the influence of the stopping-power data on the STPR, the dependence of the STPR on the ion energy, and STPRs for SOBP.

2. Materials and methods

For all our calculations we used the Monte Carlo particle transport code SHIELD-HIT (Gudowska et al 2004, Geithner et al 2006), based upon the most recent version SHIELD-HIT08 (Sobolevsky 2010). A number of improvements and new functionalities were added to SHIELD-HIT08, as documented in Hansen et al (2011a), finally resulting in SHIELD-HIT10A (Hansen et al 2011b). Here, only the relevant changes are reported. First, there is now the possibility of directly scoring the STPR of any media, described in detail in section 2.4. Apart from this, raster scan files generated by the treatment planning software TRiP (Krämer et al 2000, Krämer and Scholz 2000) can now be read by SHIELD-HIT in order to recalculate SOBPs. In this study, we present calculations from four single-field carbon ion SOBPs, listed in table 1. The width of the SOBP is defined as usual by the width in which the dose is above 95% (IAEA 2000). All SOBPs are three-dimensional dose cubes with equal side lengths. The resulting raster-scan file describes the number of particles required for each raster point and for each energy slice providing the necessary input for SHIELD-HIT to generate the radiation field for the SOBP. A ripple filter implementation based on the design described by Weber and Kraft (1999) is added to SHIELD-HIT in a similar way as specified by Bassler et al (2010b), in order to produce flat SOBPs.

The practical range, $R_p$, is defined for protons as the depth at which the absorbed dose beyond the Bragg peak or SOBP falls to 10% of its maximum value (IAEA 2000). However,
for ions heavier than protons this definition of $R_p$ is not feasible due to the pronounced dose tail of secondary particles. Therefore, the depth at which the absorbed dose beyond the Bragg peak or SOBP decreases to 50% of its maximum value is proposed and used here for ions heavier than hydrogen, i.e. $z > 1$. Also other definitions of $R_p$ have been used before as discussed in Kempe and Brahme (2008). The residual range $R_{\text{res}}$ at a depth $d$ is then defined as

$$R_{\text{res}} = R_p - d$$

and the measurement depth $d_{\text{ref}}$ at the middle of the SOBP in accord with TRS-398 (IAEA 2000).

2.1. Stopping powers and mean excitation energy

The stopping power $S$ is defined as the average energy change $dE$ of a particle per unit length $dl$ in a medium. At high energies, that is, from about 10 MeV/u up to 1 GeV/u, the mean energy loss of a charged particle to atomic electrons is well approximated by Bethe’s original theory (Bethe 1930, 1932) which treats the electromagnetic interaction in first-order quantum perturbation theory. At lower energies, however, additional higher-order terms are required in order to reproduce experimental results. The transition from the regime of quantum perturbation theory to the one permitting a classical treatment is described in Bohr’s distinguished survey paper (Bohr 1948).

A widespread formulation of Bethe’s theory summarizing all terms of the lowest-order stopping number $L_0$ was proposed by Fano (1963):

$$\frac{S}{\rho} = \frac{4\pi e^4}{m_e u^2} \frac{1}{A} Z^2 \left[ \ln \frac{2m_u v^2}{I} + \ln \frac{1}{1 - \beta^2} - \beta^2 - \frac{C}{Z} - \frac{\delta}{2} \right].$$

In equation (3), $\rho$ is the density of the medium, $m_e$ is the electron mass, $e$ and $u$ are the elemental units of the electric charge and atomic mass, respectively, $Z$ and $A$ are the atomic number and the relative atomic mass of the target medium, respectively, $v$ and $z$ are the velocity and the charge of the projectile, respectively, and $\beta = v/c$ where $c$ is the velocity of light in vacuum. The mean excitation energy of the target medium is denoted by $I$, while $C/Z$ and $\delta/2$ are the shell correction and the density-effect correction, respectively. The second and third terms in the square brackets containing $\beta$ originate from Bethe’s relativistic extension (Bethe 1932) and are often referred to as relativistic corrections. The expression in equation (3) is consistent with the first term $L_0$ of the stopping number $L$ in ICRU report 49 (ICRU 1993).

For low energies the description of the stopping powers becomes more complicated and higher-order terms of the stopping number $L$ have to be taken into account in order to correct for a number of different effects, such as the Barkas and the Bloch correction, $L_1$ and $L_2$, respectively. An effective description for the energy regime below the stopping-power maximum was provided by Lindhard and Scharff (1961) assuming a rise of the stopping power which is proportional to the square root of the particle energy.

The mean excitation energy, $I$, is a property of the medium which enters logarithmically in the stopping formula (3), and is responsible for most of the target material dependence of the stopping power. It is, on the other hand, completely independent of the properties of the projectile. According to equation (3), a larger $I$-value results in a smaller stopping power and consequently in a larger range of an ion in the medium. The $I$-values in ICRU report 49 (ICRU 1993) for protons and alpha particles (retained from ICRU report 37 for electrons (ICRU 1993)) for ions heavier than hydrogen is not feasible due to the pronounced dose tail of secondary particles. Therefore, the depth at which the absorbed dose beyond the Bragg peak or SOBP decreases to 50% of its maximum value is proposed and used here for ions heavier than hydrogen, i.e. $z > 1$. Also other definitions of $R_p$ have been used before as discussed in Kempe and Brahme (2008). The residual range $R_{\text{res}}$ at a depth $d$ is then defined as

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7 For carbon ions the energy regime from 10 MeV/u up to 1 GeV/u corresponds to ranges from 0.0427 cm up to 108.6 cm in water according to the revised tables in ICRU 73 (ICRU 2005).
were mainly taken from measurements. In ICRU report 73 (ICRU 2005), however, the \( I \)-values are mostly determined theoretically. As a result different \( I \)-values for the same material are recommended in ICRU reports 49 and 73. Obviously, this is inconsistent, since an \( I \)-value should not depend on the projectile. The differences existing between the ICRU reports highlight that the accuracy of the current employed methods to determine stopping-power data has still to be improved in order to provide a consistent target description.

2.2. Stopping powers in SHIELD-HIT

In the current implementation of SHIELD-HIT the compilation of required stopping-power data can be done in two ways which can be chosen independently for each target medium. First, stopping-power data can be calculated internally by SHIELD-HIT using a modified Bethe formula at high energies and a Lindhard–Scharff description (Lindhard and Scharff 1961) at low energies for any kind of material composition using the corresponding material-specific values for \( I, Z \), and \( A \) as discussed before in section 2.1. Second, an arbitrary stopping-power table may be read in as a formatted text file allowing for the use of, in principle, any stopping-power data which can be provided in electronic form. In this work the common open source library \textit{libdEdx} (Toftegaard et al 2010, Lühr et al 2011) which is available on-line is applied in order to provide tabulated data in formatted form from ICRU reports 49 (Berger et al 2005, ICRU 1993) and 73 (ICRU 2005, Sigmund et al 2009) as well as MSTAR (Paul and Schinner 2003).

The Bethe formula used by SHIELD-HIT is similar to the formulation in equation (3). But so far no shell corrections \( C/Z \) have been considered. These are known to be most relevant for low energies where, however, the Lindhard–Scharff description is used instead in SHIELD-HIT. Furthermore, it was demonstrated that for low energies (about 1 MeV/u), the accuracy of stopping-power data is insignificant for particle therapy (Elsässer et al 2009). The same argument holds for the higher-order term \( L_1 \). Additionally, the Bethe formula is modified in order to allow for electron capture (significant for low energies) by using an effective energy-dependent scaling of the projectile charge \( z \) by Hubert et al (1989). Currently, relativistic corrections proposed by Lindhard and Sørensen (1996) are still missing in SHIELD-HIT. Their importance increases for heavy ions with large nuclei which cannot be approximated as point-like particles. Although their relevance for particle therapy should be studied, no significant impact has been expected so far.

Due to existing inconsistencies in the stopping-power data recommended by ICRU—discussed in section 2.1—different sets of stopping powers are used in this work, all listed in table 2. Thereby, sets 1 and 2 as well as sets 4 and 5 are directly related to ICRU reports. For comparison, in set 3 the preferred \( I \)-values of Henkner et al (2009) are used while set 6 employs the frequently used data provided by MSTAR (Paul and Schinner 2003). The intended purpose of sets 1 and 2 is the attempt to describe the target media consistently with only one \( I \)-value for all ions, both with \( z \leq 2 \) as well as \( z > 2 \), applying SHIELD-HIT’s internal routine to determine the stopping power. Accordingly, set 1 uses only the \( I \)-values from ICRU report 73, \( I_{73} \) (the revised value for water, \( I_{\text{water}} = 78 \text{ eV} \), was very recently published in the erratum to ICRU 73 (Sigmund et al 2009)), while only \( I \)-values from ICRU 49, \( I_{49} \), are used in set 2. The motivation for sets 4 and 5, on the other hand, is the direct application of the recommended tabulated data which can be found in ICRU reports 49 and 73 for ions with \( z \leq 2 \) and \( z > 2 \), respectively. While set 4 uses the recently revised stopping-power data for heavy-ions on water, set 5 uses, for comparison to earlier studies of the STPR, the water data as originally published in ICRU 73. Note that the recently revised data from ICRU 73 (Sigmund et al 2009) were not employed by Henkner et al (2009).
### Table 2. Specifications for six sets of stopping-power data used in this work. The stopping-power data for the first three sets are determined internally by SHIELD-HIT (cf section 2.2) using the given values for \( I_{\text{water}} \) and \( I_{\text{air}} \), while those for sets 4–6 are directly read by SHIELD-HIT as text files in tabulated form. For the latter, two different tables per set are used distinguishing between the lightest (H and He) and heavier ions. The table specifies for each set its number, \( I_{\text{water}} \) and \( I_{\text{air}} \) in eV, the range of ions for which these data are applied, references, and if adequate additional comments. Further explanations can be found in the text.

| Set | \( I_{\text{water}} \) | \( I_{\text{air}} \) | Ion range | Reference | Comments |
|-----|------------------|------------------|-----------|-----------|----------|
| 1   | 78               | 82.8             | \( z \geq 1 \) | ICRU 73 (ICRU 2005, Sigmund et al 2009) | Using revised \( I_{\text{water}} \) Sigmund et al (2009) |
| 2   | 75               | 85.7             | \( z \geq 1 \) | ICRU 49 (ICRU 1993) | |
| 3   | 80.8             | 85.7             | \( z \geq 1 \) | Henkner et al (2009) | |
|     |                  |                  |           |           |          |
|     |                  |                  |           |           |          |
| 4   | 78               | 82.8             | \( z > 2 \) | ICRU 73 (ICRU 2005, Sigmund et al 2009) | Revised data for water Sigmund et al (2009) |
| 5   | 75               | 85.7             | \( z \leq 2 \) | ICRU 49 (ICRU 1993) | |
| 6   | 67.2             | 82.8             | \( z > 2 \) | ICRU 73 (ICRU 2005) | Only original data for water |
| 7   | 75               | 85.7             | \( z = 1 \) | ICRU 49 (ICRU 1993) | |
| 8   | 75               | 85.7             | \( z > 1 \) | MSTAR (Paul and Schinner 2003) | Charge scaling of ICRU 49 |

#### 2.3. Stopping-power ratio

The stopping-power ratio \( S_{a/b} \) between medium \( a \) and medium \( b \) is (cf TRS-398 \(^8\) (IAEA 2000)) given as a particle fluence weighted average over all primary and secondary particles. It is determined by calculating the dose ratio via the track-length fluence \( \Phi_{a,i}(E) \) of particle \( i \) in medium \( a \) as a function of the particle energy \( E \) and the mass stopping power \( S_i(E)/\rho \):

\[
S_{a/b} = \frac{\sum_i \int_{E_{\text{min}}}^{\infty} \Phi_{a,i}(E) \left( \frac{S_i(E)}{\rho} \right)_a \mathrm{d}E}{\sum_i \int_{E_{\text{min}}}^{\infty} \Phi_{a,i}(E) \left( \frac{S_i(E)}{\rho} \right)_b \mathrm{d}E}.
\]  

In equation (4), the numerator and denominator are equal except for that the mass stopping power of medium \( a \) enters in the numerator and of medium \( b \) in the denominator. An energy cutoff \( E_{\text{min}} > 0 \) may originate, e.g., from the chamber geometry. The contribution of ‘track-ends’ to the total dose deposition and to the corresponding STPR was studied in Geithner (2006). There it was concluded that they are not of relevance for light-ion dosimetry which is in contrast to electrons, where the contribution to the total deposited dose can be between 6% and 8% (ICRU 1984).

In contrast to the correct definition for the STPR of an ion field in equation (4), the ratio of stopping powers for media \( a \) and \( b \) for one particle species of energy \( E \),

\[
\frac{(S(E)/\rho)_a}{(S(E)/\rho)_b} = \frac{\left( \frac{Z}{A} \right)_a \ln[2m_e v^2/I_a]}{\left( \frac{Z}{A} \right)_b \ln[2m_e v^2/I_b]}.
\]  

\(^8\) In IAEA TRS-398 only the water-to-air STPR is explicitly defined, i.e. \( a=\text{water} \) and \( b=\text{air} \). However, this definition is also useful for other media combinations.
has often been considered as an approximation to the STPR, e.g. in Henkner et al (2009), Paul et al (2007) and IAEA (2000). The right-hand side of equation (5) is expressed by Bethe’s stopping formula as given in equation (3) but omitting corrections. Note that the ratio in equation (5), which considers only one particle species, is a function of the particle energy $E$ in contrast to the STPR in equation (4) which has a spatial dependence and takes the full energy spectra of all particles into account.

2.4. Scoring of the STPR in SHIELD-HIT

STPRs have already been obtained with SHIELD-HIT before (Henkner et al 2009, Geithner et al 2006) and only the conceptual improvements in this work are discussed in the following. The concept of virtual scoring has been introduced which now allows for a parallel detector geometry independent of any physical geometry. Therefore, there is no longer a need for introducing artificial physical geometries which lead to additional region boundaries. Furthermore, the STPRs are now determined on-line, that is, during the transport of the particles. An on-line calculation has the advantage that possible influence on the result due to the number and size of the energy scoring and energy spacing is avoided. Additionally, higher accuracy in scoring of tracks-ends can be achieved in principle.

The detector for the STPR resembles equation (4) and is implemented in the following way. When a particle traverses a bin of the STPR detector, its track-length fluence within the bin is scored and directly multiplied with $(S/\rho)_a$ of the medium $a$ in which the particle moves for the energy $(E_{in} + E_{out})/2$. $E_{in}$ and $E_{out}$ are the energies of the particle when it enters and leaves the bin, respectively. Additionally, the same track-length fluence is multiplied with $(S/\rho)_b$ of the same particle. Both quantities are summed up individually including all particles passing the bin. After a full Monte Carlo transport simulation, the two sums are divided yielding the STPR for this bin.

In this work a transport cutoff of 0.025 MeV/u is used by SHIELD-HIT which means that all particle tracks end once the particle energy becomes smaller. Consequently, the lower limit for the integration in equation (4) is given by $E_{min} = 0.025$ MeV/u having an influence on the STPR of less than 0.000 15% (Henkner et al 2009). A recent review article (Belkić 2010) discusses in some detail the impact of electrons in fast ion–atom collisions with respect to hadron therapy as well as the possibility of extending SHIELD-HIT in a way that electron tracks are also considered. This would allow for studies of the microscopic energy distribution in the target medium. Tracking of delta electrons has for example been performed with Geant4 (Taddei et al 2008) and a study comparing to this work might be of interest.

2.5. Analytic expression for the average ion energy

The stopping-power formula as presented in equation (3) for a specified combination of the projectile and the target is primarily a function of the projectile’s kinetic energy which decreases during the passage through the target medium due to the energy loss. In order to determine the average energy of the projectiles as a function of depth, a full simulation of the particle transport has to be performed. This comprises the slowing down caused by all relevant energy-loss mechanisms including elastic as well as nonelastic interactions (ICRU 2000). Thereby, nonelastic nuclear reactions produce a spectrum of particles with each particle having an individual energy distribution which is furthermore a function of the position in the medium. Consequently, it would be highly desirable to have a simple, though approximate,
analytical expression $E(d)$ for the average energy of the primary particles with initial energy $E_0$ as a function of the penetration depth $d$.

Starting with the Bethe formula, but assuming first that the expression in the square brackets of equation (3) is independent of energy, $E(d)$ can easily be expressed analytically as

$$E(d; E_0, R_p) \approx E_0 \left(1 - \frac{d}{R_p}\right)^{1/2},$$

(6)

where $R_p$ is the practical range. $R_p$ depends in general on the ion species, $E_0$, and the target material. For energies relevant in particle therapy, $R_p$ can often be approximated by $R_0$ obtained with the continuous slowing down approximation (CSDA).

In order to account for the correct energy dependence of the Bethe formula as well as nonelastic collisions, one has to allow for a more general power-law relation,

$$E(d; E_0, R_p) = E_0 \left(1 - \frac{d}{R_p}\right)^{1/k},$$

(7)

with an exponent $k$. Different values for $k$ are suggested in the literature while Kempe and Brahme (2008) proposed the use of a dimensionless transport parameter $k = E_0/R_0 S_0$ with $S_0 = S(E_0)$. A value of $k = 1.7$ fits the calculations performed with SHIELD-HIT being also compatible with Kempe and Brahme (2008) and is therefore used in this study.

2.6. Analytic expression for the STPR

In order to derive an analytic, though approximate, expression of the STPR as a function of the depth $d$ for two media $a$ and $b$, the approximation to the average energy in equation (7) can be used together with the ratio of stopping powers given in equation (5). Utilizing the non-relativistic relation $v^2 = 2E/m_p$ between the particle velocity $v$ and its kinetic energy $E$, where $m_p$ is the proton mass, one obtains the expression

$$\tilde{S}_{(a/b)}(d) = \left(\frac{Z_a}{Z_b}\right)^{\langle Z/A \rangle_a/\langle Z/A \rangle_b} \ln\left[\frac{E_0}{I_a}\right] + C(d) + \ln\left[\frac{E_0}{I_b}\right] + C(d),$$

(8)

where

$$C(d) = \frac{1}{k} \ln \left[1 - \frac{d}{R_p}\right] - 6.1291$$

(9)

and $\ln[4m_e/m_p] = -6.1291$ have been used. Similarly as in equation (4), the numerator and denominator in equation (8) are equal except for the different $I$-values and $(Z/A)$ ratios. It should be mentioned that in order to keep the expression for $\tilde{S}_{(a/b)}$ as simple as possible, its derivation has been performed without relativistic kinematics which are in principle of relevance for the highest energies used in particle therapy. Finally, the expression in equation (8) should explicitly be formulated for the water-to-air STPR

$$\tilde{S}_{(\text{water/air})}(d) = 1.11195 \ln\left[\frac{E_0}{I_{\text{water}}}\right] + 1/k \ln\left[1 - d/R_p\right] + 7.6863 \ln\left[\frac{E_0}{I_{\text{air}}}\right] + 1/k \ln\left[1 - d/R_p\right] + 7.6863,$$

(10)

being the most relevant case for dosimetry in particle therapy, with $E_0$ and $I$ in units of MeV/u and eV, respectively. For convenience, constants are expressed in numbers, i.e. $\ln[4 \times 10^6 m_e/m_p] = 7.6863$ and $\langle Z/A \rangle_{\text{water}} / \langle Z/A \rangle_{\text{air}} = 0.555076 / 0.499189 = 1.11195$ (ICRU 1984).
3. Results

In what follows, results for the STPRs of pristine Bragg peaks and SOBPs are presented. Furthermore, analytic expressions are compared to the numerical results obtained with SHIELD-HIT. For simplicity, only results for ion beams in water are considered, and STPRs are presented exclusively for water to air. Furthermore, only stopping-power set 1 of table 2 is used in order to ensure consistent results except for figure 1(b) which demonstrates the dependence of $S_{water/air}$ on the choice of the stopping-power set.

3.1. Pristine Bragg peaks

A comparison between the calculated STPR for water to air of 270 MeV/u carbon ions as a function of depth in water and the corresponding depth-dose distribution is shown in figure 1(a) focusing on the vicinity of the Bragg peak. The maximum of the STPR almost coincides with the practical range $R_p = 144.6$ mm and therefore appears to be at a larger depth than the dose maximum. The width of the STPR peak is considerably smaller than that of the dose curve. The determined height of the STPR depends to some extent on the finite spatial resolution along the beam axis. A coarse resolution leads to spatial averaging and accordingly to a lower peak height of the STPR. Note that the position of the Bragg peak and therefore $R_p$ is only influenced by the choice of stopping-power data for water.

The influence on the STPR due to the use of different stopping-power data is demonstrated in figure 1(b) for a 270 MeV/u carbon pencil beam by using all stopping-power sets 1–6 of table 2. In the plateau region, the deviations of sets 1–6 from the value 1.13 recommended by the IAEA in the TRS-398 (IAEA 2000) are within 1%. Set 2, which employs $I_{49}$ for water and air, differs the least. This is consistent since the recommendation in TRS-398 is based on the stopping-power data provided by ICRU report 49. In contrast to the recommended value 1.13, none of the calculated STPR curves is constant. However, the relative increase in the plateau region up to a depth of 130 mm ($R_{exp} \approx 15$ mm) is moderate and of the order of approximately 0.2% to 0.3%. For all sets of stopping powers, except for set 4, an increase in the STPR can be observed in the vicinity of the Bragg peak. Set 4 on the other hand shows a dip. This dip

![Figure 1](image-url)
originates mostly from the carbon ions and can therefore be attributed to the tabulated data provided in the revision of ICRU 73.

The two STPR curves calculated with sets 1 and 3—the latter was used in Henkner et al (2009)—lie virtually on top of each other in figure 1(b) although the I-values of sets 1 and 3 differ notably. This can be explained by the differences of the I-values for water and air which are very similar to 4.8 and 4.9 eV for sets 1 and 3, respectively. As expected, $S_{\text{water/air}}$ obtained with the tabulated data from ICRU 73, that is, set 4, agrees with the STPR curve obtained with $I_{\text{73}}$, set 1, in the plateau region. On the other hand, the STPR curves for sets 1 and 4 deviate around and beyond $R_p$. The use of stopping-power set 5 by Henkner et al (2009) resulted in an unphysical minimum of the STPR in the plateau region. In the current study, however, no minimum of the $S_{\text{water/air}}$ curve obtained with set 5 can be observed.

The influence of different initial energies on the STPR for carbon ion beams as a function of the residual range $R_{\text{res}}$ is shown in figure 2(a). The STPR curves as a function of $R_{\text{res}}$ are almost identical in the plateau region and therefore independent of the initial energy. Around and beyond the Bragg peak the curves are still alike, though lower initial energies lead in general to higher STPR values.

The stopping-power ratio $S_{\text{water/air}}$ as a function of $R_{\text{res}}$ for different ion beams relevant for particle therapy, H, He, Li, C, N, O, Ne, Si, and Ar, is presented in figure 2(b). Different beam energies for the individual ions have been chosen, ranging from 130 to 400 MeV/u, in order to achieve comparable penetration depths. In the plateau region, the STPRs for the different ion beams all share the same qualitative behavior which has already been discussed before in the context of carbon ions, cf figures 1(b) and 2(a). A comparison among the ions yields that decreasing STPRs at a given $R_{\text{res}}$ occur for increasing atomic numbers $z$. The decrease becomes less pronounced for larger $z$. An exception from this trend is found for H and He ions with very similar $S_{\text{water/air}}$ in the plateau. The relative difference of STPRs between the lightest and heaviest ion $z = 1$ and $z = 18$, respectively, is rather constantly about 0.15%.

Around and beyond $R_p$ ($R_{\text{res}} \lesssim 0$), the STPR seems to be larger for ions with larger $z$. However, some dependence also might originate from the different initial energies of the ion beams, as has been observed in figure 2(a). While the STPR for H ions is nearly identical to that for He ions in the plateau region, differences to all other ions with $z > 1$ are
obvious for $R_{res} \lesssim 0$. However, as discussed in section 2, the definition of the practical range $R_p$ for protons differs from that used for ions with $z > 1$ which influences—according to equation (2)—also the residual range $R_{res}$.

### 3.2. Spread-out Bragg peaks

Four different SOBPs obtained with carbon ion fields are considered with stopping-power set 1 in this study and their properties are listed in table 1. Figure 3(a) displays the depth-dose distribution (line) and the corresponding STPR (symbol) of the biologically optimized SOBP $d$. The proximal start of the SOBP region can be recognized in the STPR curve as a significant increase. Toward the distal end of the SOBP, the STPR reveals an exponential increase. As for pristine peaks in figure 1(a), the maximum of the STPR curve is reached close to $R_p$. A sharp fall off of the STPR occurs for depths $d > R_p$ which finally results in a constant STPR. Note that this qualitative description is valid for all SOBPs $a$–$d$ and is therefore independent of the specific form of the SOBP or whether it is physically or biologically optimized.

The STPRs of all four SOBPs $a$, $b$, $c$, and $d$ are compared in figure 3(b) as a function of $R_{res}$. SOBPs $a$ and $c$ share the same width but differ in $R_p$. Therefore, their STPRs as a function of $R_{res}$ are nearly identical. The STPR curves for $b$ and $d$ show a very similar behavior as $a$ and $c$ but are extended to 80 and 100 mm, respectively, according to the larger width of their SOBP region.

It should be mentioned that for SOBP $b$ a number of ripples in the STPR can be observed in the proximal SOBP region. They originate from the optimization program TRiP which assumes treatment at the SIS accelerator at Gesellschaft für Schwerionenforschung (GSI), Darmstadt, Germany. The SIS provides finite energy steps which are more coarse at the lowest energy part when no bolus is applied.

The calculated STPR and dose transverse to the beam axis at the reference depth $d_{ref} = 150$ mm (defined as middle of SOBP (IAEA 2000)) are displayed in figure 4 for SOBP $c$. The STPR is perfectly constant within the full extension of the SOBP transverse to the beam axis. A moderate increase in the STPR occurs outside the SOBP.
3.3. Analytical description of the STPR

The purpose of this section is to relate an analytical description of the STPR to the numerically obtained STPR. Thereby, it is important to keep in mind that according to the results obtained so far the STPR \( S \) (a) depends primarily on \( R_{\text{res}} \), that is, average ion energy, and (b) is qualitatively independent of the ion species.

The STPR \( S_{\text{water/air}} \) for a 270 MeV/u carbon ion beam using stopping-power set 1, as shown before in figure 1(b), which considers the full particle spectrum is compared in figure 5 to two approximations of the STPR: (i) the STPR obtained with SHIELD-HIT but ignoring the influence of produced fragments on \( S_{\text{water/air}} \) by only considering the STPR resulting from carbon ions and (ii) the analytic expression in equation (10) which approximates the STPR with a ratio of stopping powers of the primary ions with an average energy depending on \( R_{\text{res}} \). Figure 5(a) clearly shows that especially in the plateau region the absolute difference between these three curves is small. Therefore, figure 5(b) additionally shows the relative difference \( \left| S_{\text{full}} - S_{\text{appr}} \right| / S_{\text{full}} \) between the STPR for the full particle spectrum, determined according to equation (4), and the two approximations of the STPR. Both approximations reproduce \( S_{\text{full}} \) within 0.02% in the whole plateau region. Around \( R_p \) the difference can be as large as 1% and they cannot be applied beyond \( R_p \) since both approximations are based on the primary particles.

In principle, the analytical expression for pristine peaks can also be of use for the SOBP. However, since the exact weights of the superposed peaks are not always known, a simple fit as a function of \( d \) may be proposed as

\[
S_{\text{water/air}}(d) = \alpha + \beta \exp[\gamma (R_p - d)] + \delta (R_p - d)
\]

(11)

which approximates the STPR within the SOBP region and is also shown in figure 3(b). The values for the four parameters in equation (11) are

\[
\alpha = 1.12205, \quad \beta = 4.0044 \times 10^{-3}, \quad \gamma = -0.241, \quad \text{and} \quad \delta = -2.0238 \times 10^{-5}.
\]

These parameters depend on the stopping-power set and slightly on the ion species (Lühr et al 2011). Outside the SOBP region the STPR might be approximated in a similar way as it is done for pristine peaks considering the average energy of the primary ions at \( d \) which is, however, different from the case of pristine peaks. From figure 3(b) it can be observed that the fit function proposed in equation (11) clearly is in acceptable agreement with the \( S_{\text{water/air}} \) curves of the four different SOBPs.
4. Discussion

4.1. Influence of the inconsistency of ICRU stopping-power data on the STPR

It is obvious that the STPR strongly depends on the stopping-power data which are used as an input for its determination. This applies for \( R_p \) and accordingly the position of the STPR maximum. Therefore, this work focuses mainly on stopping-power data for water and air which are recommended by ICRU reports. However, even if one tries to follow these recommendations, certain inconsistencies still remain and different sets of stopping-power data—as listed in Table 2—can be deduced. In the case that the tabulated data provided by ICRU are used directly, set 4, physical quantities of the target media, e.g., the \( I \)-value, depend on whether the medium interacts with protons and helium ions or with heavier ions. Although not explicitly recommended, another approach, which is more consistent from a physical point of view, is to use the \( I \)-values of only one of the ICRU reports together with an appropriate stopping formula for all ions, i.e. with \( z \leq 2 \) as well as \( z > 2 \). This is done here for sets 1 and 2 using \( I_{73} \) and \( I_{49} \), respectively\(^{10}\).

First, the STPRs in the plateau region (\( d < R_p \)) are discussed. Figure 1(b) reveals that the STPR \( S_{\text{water/air}} \) using \( I_{49} \) for all ions, set 2, agrees best with a constant value of 1.13 as recommended in TRS-398 which is plausible since TRS-398 is based on the data of ICRU 49. \( S_{\text{water/air}} \) obtained with \( I_{73} \), set 1, is about 1% smaller compared to that obtained with \( I_{49} \), set 2, but agrees nicely with the tabulated data recommended by ICRU, set 4. Second, around \( R_p \) the STPR curves of all data sets show a distinct maximum except for that of set 4 for which a minimum can be observed. This minimum does not originate from differences in the target descriptions due to the use of ICRU 49 and 73 in set 4 but is exclusively caused by

\(^{10}\) A further option is to correct for the \( I \)-value in one of the two recommended sets of ICRU tables leading to a more consistent description of the target media. According to equation (3), this could be done in first order using the term \( 0.307075 (\alpha^2 \beta^1)/(\beta^3 \alpha) \ln [I_{49}/I_{73}] \) for correcting ICRU report 49 or its negative value for correcting ICRU report 73 (Sigmund 2010). This approach is of course not applicable in the low-energy regime where, on the other hand, the ICRU tables anyhow provide a limited accuracy only. However, this option has not been pursued in this work.
the low-energy ratio of stopping powers taken from ICRU 73. Third, beyond the peak \(d > R_p\) \(S_{\text{water/air}}\) is rather constant for all stopping-power sets with a consistent description of the target media. For sets 4 and 5 the faster decline of the heavier ions relative to the lighter ones beyond \(R_p\) leading to a transition from ICRU 73 to 49 is clearly revealed by 1(b). Therein, the latter two curves finally converge to \(S_{\text{water/air}}\) obtained with I_{49}, set 2.

The use of the out-dated standard, that is, stopping tables from ICRU 49 and 73 without the revisions of ICRU 73 for water, set 5, is not advised. Set 5 yields a STPR which is in the plateau region about 1% and 2% larger than the value 1.13 recommended by TRS-398 and the values obtained with revisions of ICRU 73 for water, set 4, respectively. It should be mentioned that the results for set 5 in figure 1(b) do not show any unphysical minimum in the plateau region as was observed before in Henkner et al (2009) and Paul et al (2007). There, the unphysical structure was attributed to the use of different stopping-power data from ICRU 49 and 73 for different ions. However, in this work it was possible to reproduce the exact shape of the curve as shown in figure 2 of Henkner et al (2009) by using the stopping-power data of ICRU 49 and 73 with only three digits instead of the four digits provided by the tables. Hence, the present findings clearly contradict the statement in Henkner et al (2009) claiming that the unphysical structure results from the use of two different sources of stopping-power data, namely ICRU 49 and 73. Instead, we can conclude that the reason for the unexpected behavior observed in Henkner et al (2009) is simply errors resulting from a too coarse rounding in the applied stopping-power data tables and is not caused by a combined use of ICRU 49 as well as 73.

4.2. Dependence of the STPR on the average ion energy

One quintessence of this work is that the STPR for a given set of stopping-power data is mostly determined by the average energy of the ions, rather than their initial energy or their charge which is nicely confirmed by figure 2. Figure 5 shows furthermore that for \(d < R_p\) the STPR is completely dominated by the STPR of the primary ion species and the relative deviation is of the order of 0.02%. In a next step, the STPR of the primary ions can be nearly exactly reproduced using the ratio of stopping powers, as expressed in equation (5), for the average energy of the primary ions at a depth \(d\). Since the average energy can be rather accurately expressed as a function of \(d\), in a final step this energy function is used together with equation (5) to formulate the analytical expression of the STPR in equation (10). The analytical expression reproduces the STPR of the primary ions very well and deviates accordingly also in the order of 0.02% from the correct STPR obtained with the complete particle spectrum.

Note that the key advantage of the proposed analytical expression is its flexibility. It is not restricted to a specific set of stopping-power data. Consequently, it could be easily adopted to any new recommendation by ICRU. It is not restricted to specific primary ions and only their average energy as a function of depth is required. It is not restricted to a specific combination of target materials such as water and air being in the focus of this work. For example, it can be straightforwardly used for the STPR for water to tissue and air to tissue which would be of interest when comparing dose to medium with dose to water as recently discussed by Paganetti (2009).

These findings lead to two central insights. First, in contrast to the presumption in TRS-398, the knowledge of the whole particle spectrum is not of practical importance for the plateau and peak region\(^{11}\). The STPR can be simply approximated with a relative deviation much smaller than the uncertainties of all available stopping-power data. On the other hand, the

\(^{11}\)The relevance of the whole particle spectrum for determining the STPR increases if for some secondary particles different stopping-power data are employed, e.g. ICRU 73 and 49.
secondary particles are of central importance beyond $R_p$ where the primary ions are ceased. However, it has to be stressed that these conclusions do not consider the impact of secondary particles originating from the use of passive scattering methods such as edge-scattered protons theoretically studied in Titt et al (2008). An explicit inclusion of this kind of secondary particles and their impact on the STPR might call for a further detailed study. Second, it is not necessary to study STPRs for all ions independently since they can be approximated in the same way as proposed in equation (8). The small quantitative differences among the STPRs of the various ions shown in figure 2(b) may be explained best with the different average energies at a given $R_{res}$.

4.3. STPRs for SOBPs

Clinical applications require a relatively uniform dose to be delivered to the volume to be treated and for this purpose the ion beam has to be spread out both laterally and in depth. With respect to the STPR of SOBPs, the gist of this work is that the qualitative behavior of the STPR is hardly dependent on the specific spatial form of the SOBP, its depth in the medium, and whether it is optimized for a homogeneous physical dose or relative biological dose.

This statement is nicely verified in figure 3(b) where $S_{\text{water/air}}$ is displayed as a function of $R_{res}$ for four SOBPs specified in table 1. In order to understand the observed uniform behavior of the STPR, one has to keep in mind that a SOBP is a superposition of Bragg peaks of different intensities and $R_p$ which is usually constructed from the distal end, i.e. $R_{res} = 0$, toward the proximal start. Consequently, the properties of the SOBP up till a residual range $R_{res}$ are only weakly influenced by the properties of the SOBP for larger $R_{res}$. It is therefore possible and practical to propose a fit to the STPR $S_{\text{water/air}}$ for the SOBP region, as it is done in equation (11) for carbon ions and set 1. A general drawback of the fit function compared to an analytical expression is that the parameters of the former explicitly depend on the ion species and stopping-power data. In analogy to the findings for pristine peaks, quantitative differences can be expected for ion species other than carbon ions. However, a detailed study of a number of other ions is beyond the scope of this paper and might be addressed elsewhere (Lühr et al 2011). The qualitative dependence of $S_{\text{water/air}}$ on the stopping-power set is similar as discussed before for the pristine peaks. Accordingly, the quantitative difference between $S_{\text{water/air}}$ obtained with sets 1 and 4 is due to the two features observed for set 4, namely the minimum at $R_p$ and the strong increase of the STPR beyond $R_p$ caused by the ICRU 49 tables for protons and helium.

In TRS-398 reference conditions for the determination of absorbed dose for ion beams are specified. The reference depth $d_{\text{ref}}$ for calibration should be taken at the middle of the SOBP, at the center of the target volume. It can be seen in figure 4 that a positioning error of a dosimeter transverse to the beam axis has no relevance on the STPR as long as the position is within the SOBP. This is plausible since the average energy of the ions should be the same at the same depth. A misalignment along the beam axis, on the other hand, may have an influence as seen in figure 3. The influence is largest for a SOBP with small width, for which the gradient of the STPR is largest, and becomes smaller for large widths. Therefore, an extended SOBP might be recommended for accurate dose measurements in a practical quality-assurance setting. The total variation of the STPR along the beam axis observed in figure 3(b) is of the order of 0.8%. Note that the current study assumes that besides the ripple filter no range compensator is present in the considered ion beam, i.e. active spot scanning is assumed. Uncertainties originating from the use of range compensators were recently addressed in Fontenot et al (2008).
5. Conclusions

Calculations of the water-to-air stopping-power ratio (STPR) $S_{\text{water}/\text{air}}$ using the Monte Carlo transport code SHIELD-HIT10A are performed for different ions in a range of $1 \leq z \leq 18$. The STPR is determined on-line considering the track-length fluence spectra of all primary and secondary particles as recommended by IAEA in TRS-398. In addition to providing accurate quantitative results, the focus of this work is put on a thorough qualitative understanding of the dependences of the STPR and the relevance for particle therapy.

STPRs obtained with different sets of stopping-power data recommended by ICRU (1993, 2005), including the very recently revised data for water (Sigmund et al. 2009), are compared with the value 1.13 recommended for $S_{\text{water}/\text{air}}$ in TRS-398 (IAEA 2000) resulting in deviations of the order of 1% in the plateau region. The change of the STPR due to the contribution of secondary particles is only of the order of 0.02% for pristine peaks in the plateau region and up to the Bragg peak. It can be shown that for a given set of stopping-power data, the STPR at a residual range $R_{\text{res}}$ is mostly determined by the average energy of the primary ions, rather than their initial energy or their charge $z$. A convenient analytical expression for the STPR as a function of depth in water is proposed for the plateau region up to the Bragg peak which deviates in this region by about 0.02% from the obtained results for $S_{\text{water}/\text{air}}$. The most valuable property of the analytical formula is its flexibility. It is in principle not restricted to any specific ion, stopping-power data, combinations of target media, or initial ion energies. For the case of spread-out Bragg peaks (SOBPs), it can be concluded that the qualitative behavior of the STPR is hardly dependent on the specific spatial form of the SOBP, its depth in the medium, and whether it provides a homogeneous physical dose or relative biological dose. A fit function is provided to approximate the STPR within the SOBP region for carbon ions.

Finally, it can be stated that no further theoretical studies of STPRs heading only for higher accuracy are expedient, as long as no consistent set of relevant stopping-power data for all ions is recommended, preferably with smaller uncertainties.

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