

GENERALIZED EMPIRICAL EQUATION FOR THE EXTRAPOLATED RANGE OF ELECTRONS IN ELEMENTAL AND COMPOUND MATERIALS

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COLEÇÃO PTC
Devolver no Balcão de Empréstimo

Abstract

The extrapolated range R_{ex} of electrons is useful for various purposes in research and in the application of electrons, for example, in polymer modification, electron energy determination and estimation of effects associated with deep penetration of electrons. A number of works have used empirical equations to express the extrapolated range for some elements. In this work a generalized empirical equation, very simple and accurate, in the energy region 0.3 keV - 50 MeV is proposed. The extrapolated range for elements, in organic or inorganic molecules and compound materials, can be well expressed as a function of the atomic number Z or two empirical parameters Z_m for molecules and Z_c for compound materials instead of Z .

1. INTRODUCTION

In electron beam applications, such as curing, polymer modification, sterilization of medical supplies or food decontamination, we need to estimate the depth dose curves in organic and compound materials to pre-set accelerator parameters in order to achieve the best dose uniformity.

An easy way to do this in current irradiation services is lacking and it seems to us that if we could find an analytical expression for this purpose, it would be dependent on the extrapolated or practical range.

Kobetich and Katz [1,2] and Tabata and Ito [3] formulated expressions for the depth dose curves for several absorbers, using the functional form of Weber's [4] extrapolated range-energy relation for aluminium. Instead of R_{ex} , Kobetich and Katz [2] have taken the characteristic thickness $R_{0.05}$ proposed by Dupouy [5], defined as the thickness at which the transmission coefficient has fallen to 5 %, but they employed the functional form by Weber [4]. On the other hand, Tabata *et al.* [3,6] used only the R_{ex} concept.

The present work uses the functional form of Weber relation (Eq. 1).

$$R_{ex} = AW[1 - B/(1 + CW)] \quad (1)$$

where: R_{ex} : is the extrapolated range in aluminium,
 W : is the monoenergetic energy of electrons, and
 A, B, C are numerical constants.

We also employed the characteristic thickness concept, taking data of transmission curves for heavy elements.

2. EXPRESSIONS

2.1. Expression for $R_{ex}(E, Z)$

The extrapolated or practical range R_{ex} of monoenergetic electrons in the energy region 0.3 keV – 50 MeV for the elemental absorbers was found to be well expressed by Eq. (2):

$$R_{ex} = 1.41 \frac{Z^{0.68}}{Z + 1.8} E \left[1 - \frac{0.985}{1 + Z^{1.9} \cdot 10^{-5} + 3.1E} \right] - Z^{0.45} E^{2.12} \cdot 10^{-4} \quad (2)$$

where, R_{ex} : is the extrapolated or practical range (g/cm²),
 E : is the incident electron energy (MeV), and
 Z : is the atomic number.

2.2. Expression for Z_m

The same expression applies to organic or inorganic molecules since we express Z by a empirical parameter Z_m defined by Eq. (3):

$$Z_m = \frac{\sum_i N_i Z_i + 4N_H}{\sum_i N_i} \quad (3)$$

where, N_i : is the number of atoms i in the molecule, excluded the hydrogen atoms,
 Z_i : is the atomic number of atom i , and
 N_H : is the number of hydrogen atoms in the molecule.

TABLE I. SOME VALUES OF Z_m or Z_c

Material	Composition	Z_m or Z_c
Air	0.755 N; 0.232 O; 0.013 Ar	$Z_c = 7.27$
Polyethylene terephthalate	(H ₈ C ₁₀ O ₄) _n	8.85
Polyacrylonitrile	(H ₃ C ₃ N) _n	9.25
Polycarbonate	(H ₁₄ C ₁₆ O ₃) _n	9.26
Acrylonitrile-Butadiene-Styrene - ABS	0.68 (H ₃ C ₃ N); 0.07 (H ₆ C ₄); 0.25 (H ₈ C ₈)	9.6
Cellulose Triacetate - CTA	0.85 (C ₁₂ H ₁₆ O ₈); 0.15 (C ₁₈ H ₁₅ PO ₄)	9.93
Aluminium oxide	Al ₂ O ₃	10.0
Polybutadiene	(H ₄ C ₄) _n	10.0
Polystyrene	(H ₈ C ₈) _n	10.0
Cellulose	(H ₁₀ C ₆ O ₅) _n	10.54
Polymethylmethacrilate - PMMA	(H ₈ C ₅ O ₂) _n	11.14
A-150 Tissue Equivalent Plastic	0.064 H; 0.534 C; 0.027 N; 0.030 O; 0.167 F; 0.177 Ca	$Z_c = 11.8$
6.6 Nylon	(H ₁₁ C ₆ NO) _n	11.9
Polyvinyl - alcohol	(H ₄ C ₂ O) _n	12.0
Polyvinyl chloride - PVC	(C ₂ H ₃ Cl) _n	13.66
Polyethylene	(H ₄ C ₂) _n	14
Polypropylene	(H ₆ C ₃) _n	14
Ethanol	C ₂ H ₅ OH	14
Water	H ₂ O	16

2.3. Expression for Z_c

For compound materials, Z is replaced by Z_c expressed by Eq. (4):

$$Z_c = \frac{\sum_i \frac{f_i}{A_i} Z_i + 4f_H}{\sum_i \frac{f_i}{A_i}} \quad (4)$$

where, f_i : is the fraction by weight of atom i , excluded the hydrogen atoms,
 f_H : is the fraction by weight of hydrogen atoms, and
 A_i : is the atomic mass of atom i .

2.4. Comments

Relations (3) and (4) for Z_m or Z_c are the average content of electrons per atom, excluding the hydrogen and inserting their electrons in the media, as if they were four times more effective than the electrons belonging to the other atoms.

We can not give any physical meaning of this interpretation for Z_m or Z_c but, as it is well known, the electron or hydrogen content affects directly the energy absorption ratio (stopping power) due to inelastic electron-electron collisions. Becker *et al.* [7] showed that commercial plastics and elastomers can be ordered according to their decreasing extrapolated range by ranking them in the increasing ratio of the number of hydrogen atoms to the number of other atoms in the molecule. Table I shows some materials ordered by Z_m or Z_c value and this order is the same as Becker's [7].

In the generalized empirical Eq. (2), the term $Z^{1.9} \cdot 10^{-5}$ actuates only for high Z and for electron energies below 100 keV, and it was inserted to increase the extrapolated range for heavy elements in this region of energy, because the stopping power decreases due to elastic electron-atom collisions. Then, for light elements (Z , Z_m or $Z_c < 20$) this term can be discarded.

On the other hand, the second term in Eq. (2) is a correction related to radiation energy losses (bremsstrahlung production), and can be neglected for low Z , Z_c or Z_m materials at energies below 10 MeV (for Al, $Z=13$ and for 10 MeV, this correction is less than 1%). Then, for $E \leq 10$ MeV and light materials, the following Eq. (5) can be used:

$$R_{\alpha} = 1.41 \frac{Z^{0.68}}{Z+1.8} E \left[1 - \frac{0.985}{1+3.1E} \right] \quad (5)$$

TABLE II. SOURCES OF DATA

Ref.	Z / absorber	Ref.	Z / absorber
1	air-13-29-79-82	13	6-13-29-47-73-92
2	4-13-29-82-Polystyrene	14	4-13-29-47-79
8	6-13-79	15	water
9	13	16	6-13-29-48-82
10	13-47-50-79-82	17	4-6-13-29-47-79-92
11	13	18	Al ₂ O ₃
12	4-29-47-79	19	water

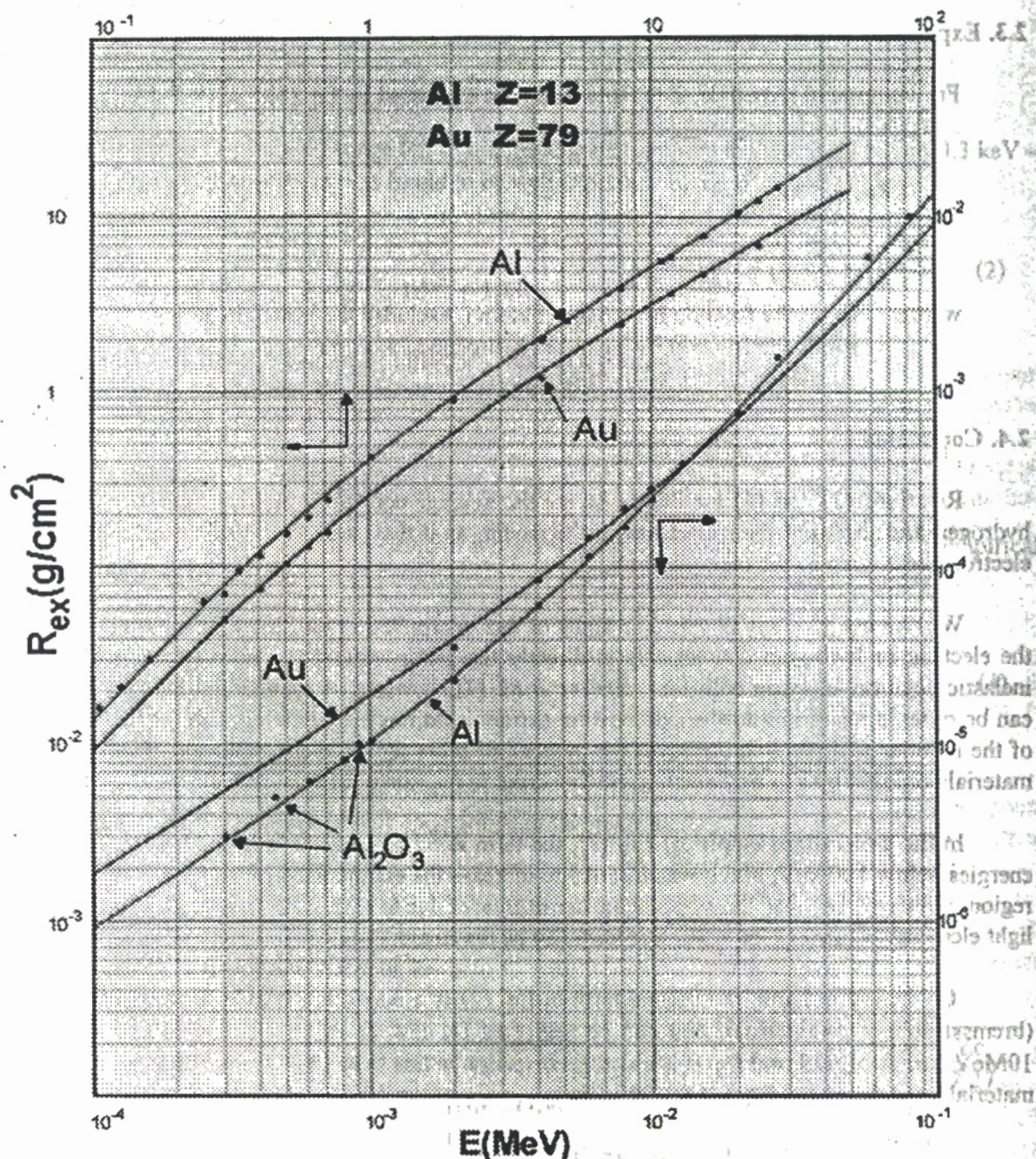


FIG. 1. $R_{ex}(E)_{Z=13}$ and $R_{ex}(E)_{Z=79}$. Lines, Eq. (2); points, experimental data.

This is Weber's Eq. (1) where the constants A, B and C are:

$$A = 1.41 \frac{Z^{0.68}}{Z + 1.8}; \quad B = 0.985; \quad \text{and} \quad C = 3.1$$

3. SOURCES OF DATA

The sources of data used are indicated in Table II. Despite the large fluctuation in the experimental data verified this does not affect so much our work for a good fitting because the simplicity of the R_{ex} expression offers the possibility of instant graphic display in the computer screen of the functions $R_{ex}(Z)$ or $R_{ex}(E)$.

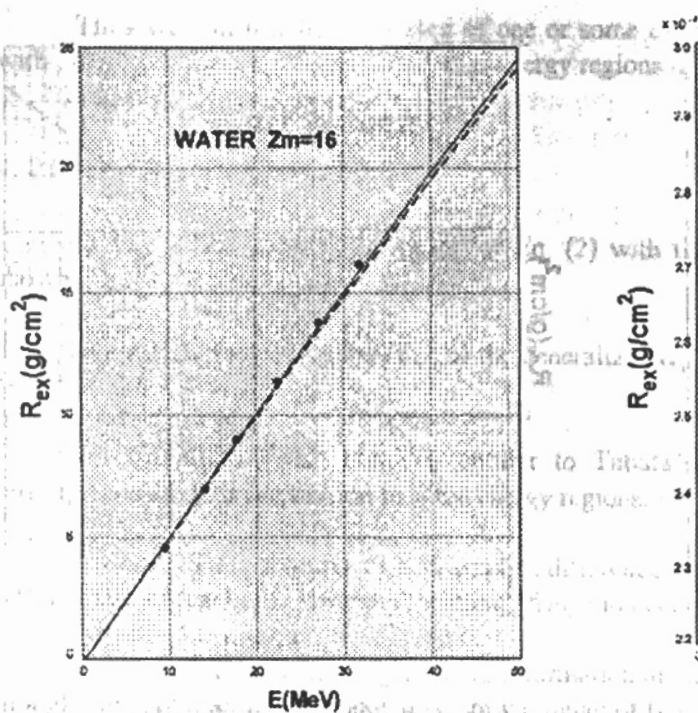


FIG. 2. $R_{ex}(E)_{water}$ Line, Eq. (2); traces, Monte Carlo analytical fit from Tabata et al [19]; points, experimental data [15].

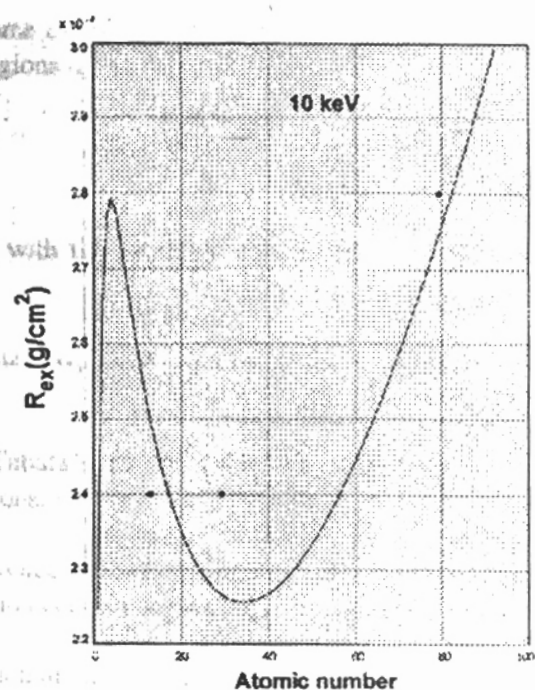


FIG. 3. $R_{ex}(Z)_{E=10keV}$ Line, Eq. (2); points, experimental data.

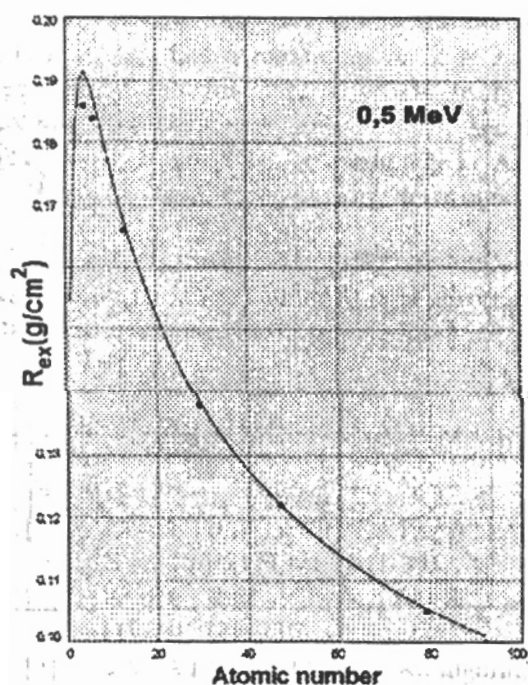


FIG. 4. $R_{ex}(Z)_{E=0.5MeV}$ Line, Eq. (2); points, experimental data.

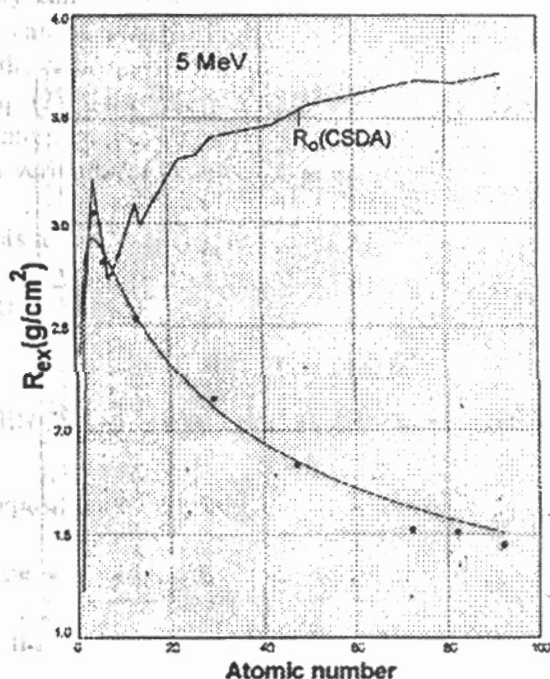


FIG. 5. $R_{ex}(Z)_{E=5MeV}$ Continuous line, Eq. (2); dashed line, $r_0(cstda)$; points, experimental data.

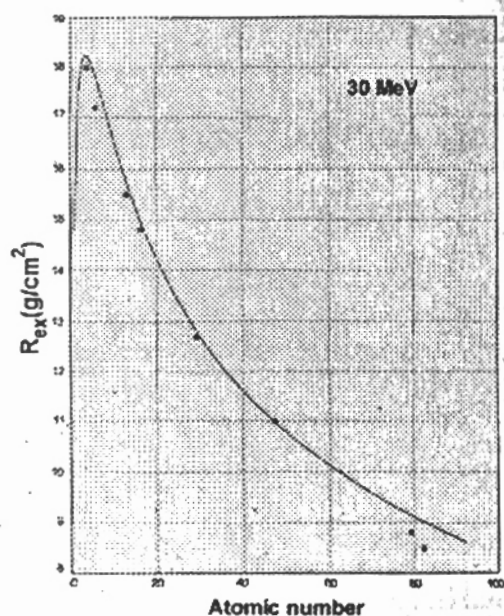


FIG. 6. $R_{ex}(Z)_{E=30\text{MeV}}$. Line, Eq. (2); points, experimental data.

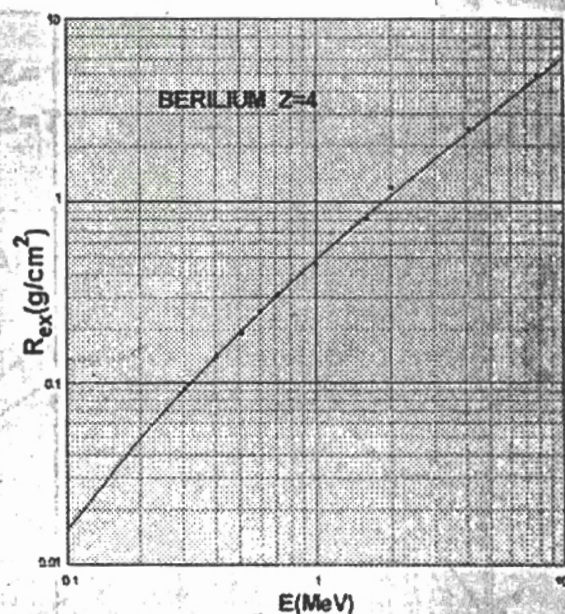


FIG. 7. $R_{ex}(E)_{Z=4}$. Line, Eq. (5), points, exper. data Refs. [2,12,14]

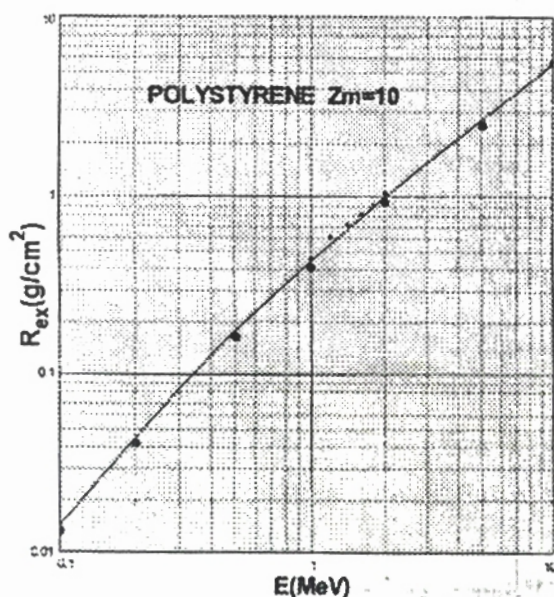


FIG. 8. $R_{ex}(E)_{Zm=10}$. Line, Eq. (5); small points, exp. data [2]; larger points, calculated by scaling law [20] between $R_{ex}(\text{water})$ and $r_0(\text{csda})$.

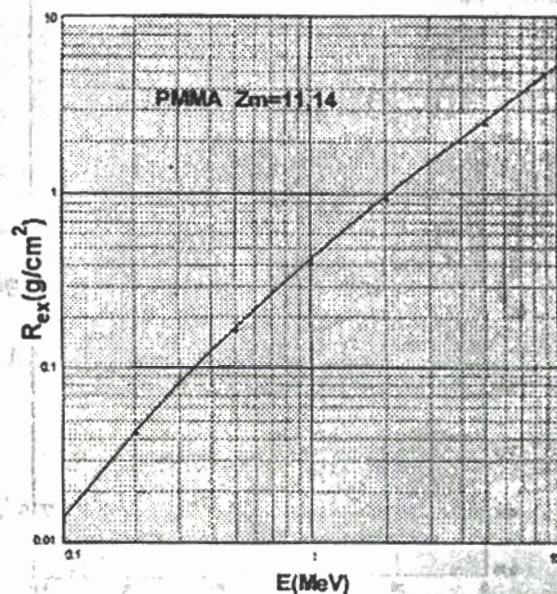


FIG. 9. $R_{ex}(E)_{Zm=11.14}$. Line, Eq. (5); points, calculated by scaling law [20] between $R_{ex}(\text{water})$ and $r_0(\text{csda})$.

Thus we can test the relevance of one or some experimental results by their level of agreement with other absorbers data or data in other energy regions of the same absorber.

4. RESULTS AND COMMENTS

In Fig. 1 the general agreement of Eq. (2) with the available data for aluminium and gold is shown.

The relative rms deviation δ_{rms} of the generalized equation from these data in all the range is: 5.6 % for Al and 4.4 % for Au.

For aluminium, this result is similar to Tabata's equation [6] that gives 6.5 % and is a consequence of data fluctuation in some energy regions.

For gold, Tabata found 13.8 % and this difference is due to the fact that our equation fits the data better, for energies below 100 keV, without change in accuracy for distinct absorbers.

These deviations can not give more information about accuracy but for absorbers with good and enough data, like aluminium and water in the range of 0.5 – 30 MeV, the deviation is 2 % or less as it can be seen in Fig. 2 for water. In this figure, Eq. (2) was plotted against the experimental and the Monte Carlo results. We plotted the analytical fit of Tabata et al. [19] for the extrapolated range of water that gives the best accordance with present Monte Carlo codes. The agreement is very good and it seems that Eq. (2) lies closer to the experimental data.

About the general accuracy of Eq. (2), we believe that it is better than 4 % for any absorber in all the energy range. Only for H and He, the accuracy can be poorer because Eq. (2) for $E=\text{constant}$, $R_{ex}(Z)_{E=\text{constant}}$ has a maximum for $Z \cong 3.8$ as it can be seen in Figs 3 to 6, and we did not find experimental data for these absorbers. In figure 5, the csda range [20] was included to show the same maximum for beryllium, $Z=4$. We also see that Eq. (2) gives values 8 % higher for He and 100 % higher for hydrogen than the csda range r_0 . As r_0 is interpreted as the mean path length, we can not have $r_0 < R_{ex}$ or the continuous-slowing down is no longer verified, for these two lightest elements.

In Fig. 3, the increase in R_{ex} for heavy elements in low energy range is shown. Figures 7, 8 and 9 show the equation (5) applied to light absorbers and energy below 10 MeV, plotted against experimental data or data estimated by a scaling law conform ICRU - 35 [20].

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