CALCULATION OF THE MASS STOPPING POWERS OF MEDICAL, CHEMICAL, AND INDUSTRIAL COMPOUNDS AND MIXTURES

by

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We developed a new version of the X-PMSP program for estimating mass stopping powers in charged particle radiotherapy, shielding of nuclear reactors and particle accelerators, and medical and energetic radioisotope production. Accordingly, we calculated the mass stopping powers of important medical, industrial, and chemical compounds and mixtures defined by International Commission on Radiation Units and Measurements using the X-PMSP program, to contribute to the existing literature and compared our results with those from the National Institute of Standards and Technology database. The application of this program, for particles in the energy range 10-50 MeV, will be especially important in the production of medical radioisotopes, as it reduces the maximum error rate to <5 % for proton, and to ~1.6 % for alpha particles. Furthermore, the maximum error rates in charged particle radiotherapy, at the energy range 1-250 MeV, are ~8.2 % for protons, and ~3.0 % for alpha particles.

Key words: stopping power, shielding material, medical material

INTRODUCTION

Particle accelerators and nuclear reactors are commonly used in industrial, medical, and space applications, such as medical radioisotope production in nuclear medicine [1-4], energy production in nuclear power plants, and heat energy and electricity production in the radioisotope thermoelectric generators (RTG) of spacecraft and space probes [5-7]. The shielding of particle accelerators and nuclear reactors is important for the safety of human health and environment. For optimal shielding of charged particles in the medium energy region, the chosen material needs to be best suited. For this purpose, the energy loss of charged particles inside the material, needs to be determined, based on the mass stopping powers of elements, compounds, and mixtures for the charged particles.

In addition to shielding, the mass stopping power is used to calculate the yield of radioisotope produced in particle accelerators, such as linear and circle accelerators, to determine the optimal radioisotope production [1-3, 6, 7]. In particular, in the energy region 1-100 MeV, the yield calculations of medical positron emission tomography (PET), single-photon emission computerized tomography (SPECT), and therapeutic radioisotopes produced by linear accelerators, synchrotrons and cyclotrons, are crucial to obtain optimal results [1]. As reported in the literature, there are many nuclear reaction processes to produce medical and industrial radioisotopes, including deuteron, triton and helium-3-induced reactions, in addition to proton and alpha particle-induced reactions. Unfortunately, the estimation of yields of deuteron, triton and helium-3-induced reactions, is poor because of the lack of methods that would provide accurate determination of the mass stopping powers of deuteron, triton, and helium-3 charged particles. Therefore, we developed the X-PMSP 2.0 program that can overcome such deficiencies in nuclear reactions in the energy region 1 MeV-1 GeV.

Radiation therapy with charged particles has received more attention than ionizing radiation therapy, or conventional radiation therapy (gamma radiation or X-ray) because of the damage to healthy tissues, such as the brain, eyes, and lungs, caused by gamma rays and X-rays, in conventional radiation therapy. However, in charged particle radiotherapy, the acceleration of particles, such as protons and alpha particles, by particle accelerator, is needed for bombarding the material. The determination of optimum incident energy of a charged particle, for human body tissues, is thus vital in charged particle radiotherapy. Mass stopping powers are used to determine the penetration range of ion beams with charged particles, such as proton and alpha particles. If the stopping powers for charged particle ion beams delivered to the human tissues, such as the brain and eye cancers, is unknown, the radiations can damage both cancer and healthy cells. Therefore,

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the stopping powers of each type of tissue and organ, for charged particle ion beams, should be accurately determined. The database of X-PMSP 2.0 includes standard parameters determined by International Commission on Radiation Units and Measurements (ICRU) for main body tissues, *e. g.*, the brain, lungs, blood, and muscles. Non-listed tissues, such as tumor, can also be entered into the program, by the users, for calculating their stopping power. Therefore, this program can potentially overcome the deficit in charged particle radiotherapy.

Although the mass stopping power can be calculated using the previous version of this program, X-PMSP 1.0 [2, 8], the new version can also calculate the mass stopping powers of compounds and mixtures, in addition to elements. Information on most medical, chemical, and industrial compounds and mixtures is present in the database of the new program. The program can also calculate for new compounds and mixtures prepared by the user, using just their chemical formulae. The previous version of X-PMSP has effectively been used for yield calculations of nuclear reactions in the production of medical radioisotopes used in PET [1], radiation therapy, and radioisotope production using particle accelerator [2, 3, 6, 7]. Therefore, in this work, we expanded the use of the X-PMSP program for the calculations for compounds and mixtures via two methods.

MATERIALS AND METHODS

Theoretical framework

To estimate the mass stopping power of elements, compounds, and mixtures for the charged particles, the following formula can be used for soft and hard collision

$$\frac{\mathrm{d}E}{p\mathrm{d}x} \quad 0.3071\frac{Zz^2}{A\beta^2} \quad 13.8373 \quad \ln \frac{\beta^2}{1 \quad \beta^2} \quad \beta^2 \quad \ln(I) \quad \frac{\delta}{2} \tag{1}$$

where Z and z represent the proton number of the target and the atomic number of the incident particle, respectively, A – the mass of the target, $\beta(v/c)$ – the velocity of the incident particle [9], and I is the mean excitation potential of the medium for materials, which was obtained from the quantum mechanical approaches and the experimental data given by Paul and Schinner [10]

$$\begin{aligned}&(\mathrm{i})\, I \quad 19.0\,\mathrm{eV}\,(Z \quad 1)\\ &(\mathrm{ii})\, I \quad 11.2 \quad 11.7\ Z\,\mathrm{eV}\,(2 \quad Z \quad 13)\\ &(\mathrm{iii})\, I \quad 52.8 \quad 8.71\ Z\,\mathrm{eV}\,(13 \quad Z)\end{aligned} \tag{2}$$

In eq. (1) δ including three situations for different X {log[β β values, represents the density effect correction calculated as follows

$$\begin{aligned}&(\mathrm{i})\,\delta(X) \quad 4.6052X \quad a(X_1 \quad X)^m \quad C \quad (X_0 \quad X \quad X_1)\\ &(\mathrm{ii})\,\delta(X) \quad 4.6052X \quad C \quad (X \quad X_1)\\ &(\mathrm{iii})\,\delta(X) \quad \delta(X_0)\ 10^{2(X \quad X_0)} \quad (X \quad X_0)\end{aligned} \tag{3}$$

where a, X_1, X_0, and C are constants of the medium [11].

To calculate the mass stopping power of 98 elements in the energy range of 1-1000 MeV, the X-PMSP 1.0 program was published by a visual interface in C# [12]. The new version of the program X-PMSP 2.0 can calculate the mass stopping powers of elements, as well as medical, industrial, chemical compounds and mixtures, in the energy region 1 MeV-1 GeV, for any increase of energy interval. The new version includes two methods (method 2 and method 3) for compounds or mixtures, as given below. In total, the program contains three sections, which can be selected based on the purposes:

(i) *Elements*: This section includes 97 different elements from hydrogen (Z = 1) to berkelium (Z = 97), in addition to hydrogen (liquid) and carbons (graphite; ρ = 2.0 gcm^{-3} and 1.7 gcm^{-3}, respectively). Density effect parameters for elemental substances used in eq. (3) were obtained from the data reported by Sternheimer *et al*. [11]

(ii) *Notable Compounds and Mixtures*: The well-known 180 chemical compounds and substances of biological interest, including 167 solid or liquid and 13 gaseous compounds and mixtures, are included. The density effect parameter and the mean excitation potential of the medium of these compounds and mixtures, were obtained from the data reported by Sternheimer *et al*. [11]

(iii) *New Compounds and Mixtures*: For any compound or mixture defined by the user, the mass stopping power can be calculated using the below equations. Here, Paul and Schinner's approach [10] in eq. (2) was used for the mean excitation potential of the medium I in compound or mixtures, instead of I data reported by Sternheimer *et al*. [11]. In addition, we used the assumption of Bragg's and Kleeman rule [13] to calculate for compounds or mixtures as follows:

$$W_i \quad \frac{N_i A_i}{{}_j N_j A_j} \tag{4}$$

$$\frac{\mathrm{d}E}{\rho\mathrm{d}x}_{\mathrm{comp.}} \quad {}_i W \frac{\mathrm{d}E}{\rho\mathrm{d}x}_i \tag{5}$$

where W_i containing N_i atoms is the weight fraction of an element, and A – the atomic weight.

The ASTAR and PSTAR databases

The ASTAR and PSTAR databases of National Institute of Standards and Technology (NIST) [14] have listed the mass stopping powers of 74 materials, including some elements, compounds, and mixtures, for proton and helium ion tabulated in ICRU Report 49 in 1993 [15]. These databases were developed by members of a report committee sponsored by ICRU to fulfill an increasing need for knowledge about the mass stopping powers and ranges. These databases have been constantly updated by NIST, based on new theoretical data obtained from computer codes and experimental data. For example, the mass stopping power data of graphite, air, and water have been re-evaluated by a committee of the ICRU (ICRU Report 90 in 2014) [16]. Thus, NIST's ASTAR and PSTAR databases have the most comprehensive data on mass stopping powers.

Due to points mentioned above, the calculated results of X-PMSP 2.0 were compared with the ASTAR and PSTAR's results, and the obtained results are presented in figs. 1-3.

RESULT AND DISCUSSION

To analyze and discuss the accuracy of the calculated results, the mass stopping powers of some medical, chemical, and industrial compounds and mixtures, were calculated using X-PMSP 2.0 and compared with the results of the NIST databases. For this purpose, we choose selected different human body tissues, *e. g.*, blood, brain, lungs, bones (compact) and muscles (skeletal), and chemical and industrial substances, including aluminum oxide (AlO), glass (borosilicate or Pyrex), polyethylene, and propane, as well as air.

The mass stopping powers of these materials for proton (p), deuteron (d), triton (t), helium-3 (He-3), and alpha ( ) particles, were obtained using the program and compared with ASTAR and PSTAR database as shown in figs. 1-3. Unfortunately, the mass stopping powers for deuteron, triton and helium-3 induced particles, are not available in the literature; hence, only the mass stopping powers of protons and alpha particles could be compared. The calculations of mass stopping powers for deuteron, triton and helium-3 induced particles, in radioisotope production applications, are indispensable for yield calculations, but, there is a wide deficiency in determining their mass stopping powers. To overcome this deficiency, X-PMSP 2.0 will be useful, especially in the radioisotope production via particle accelerator. On the other hand, the previous version of X-PMSP has been successfully implemented, for most radioisotope productions, in medical and energy fields [1-3, 6, 7].

Calculation of the mass stopping powers of medical substances

The calculated mass stopping powers of blood, bone, brain, lung and muscle, for proton, deuteron, triton, helium-3, and alpha particles, based on the standards defined by ICRU for human tissues and organs, are presented in fig. 1, together with the results of ASTAR and PSTAR databases, which do not include the mass stopping powers of blood, lung and brain. For muscle and bone tissues, the calculated results were consistent with both ASTAR and PSTAR data. In addition to the stopping powers for proton and alpha particles, those for deuteron, triton, and helium-3, were calculated to contribute to the literature. The mass stopping powers of alpha particles and helium-3 are higher than those of other particles, due to the presence of two protons in the nucleus. When taking the mean error rates of the stopping powers of medical substances into account, the maximum error rates between the calculated curves and NIST curves, in the energy range 1-5 MeV, reach ~2.42 % for protons. This result indicates that X-PMSP 2.0 is useful for calculating the mass stopping powers of the lung and bone. Table 1 shows that the mean error rate is 1 % for protons, and a similar rate is also found for alpha particles at 10-50 MeV (tab. 2). The energy interval for the production of radioisotopes used in PET and SPECT is in the range 1-50 MeV, wherein the mass stopping power results, obtained using the new program for both proton and alpha particles, showed a low error rate. Moreover, the program is suitable for charged particle radiotherapy at 1-250 MeV, especially for alpha particles.

Calculation of the mass stopping powers of chemical and industrial substances

The mass stopping powers of AlO, glass, polyethylene, and propane, for p, d, t, He-3 and α particles, were calculated using X-PMSP 2.0, and the obtained results were compared with those from the NIST databases. The calculated results of stopping powers for both proton and alpha particles were in good agreement with the ASTAR and PSTAR data. The AlO demonstrated the lowest stopping power, compared with that of the other substances. Tables from the reports of Sternheimer *et al.* [11] were utilized in the stopping power calculations in the fig. 2, for determining the mean excitation potential of the medium and the density effect parameters. The mean error rates corresponding to different energy ranges are presented in tabs. 1 and 2. The chemical and industrial substances have an error rate of 2 % for protons induced at 5-10 MeV, whereas that of 8.2 % for protons and of 3.1 % for alpha particles induced at 1-250 MeV. Thus, this program is suitable for use at 1-1000 MeV for al-

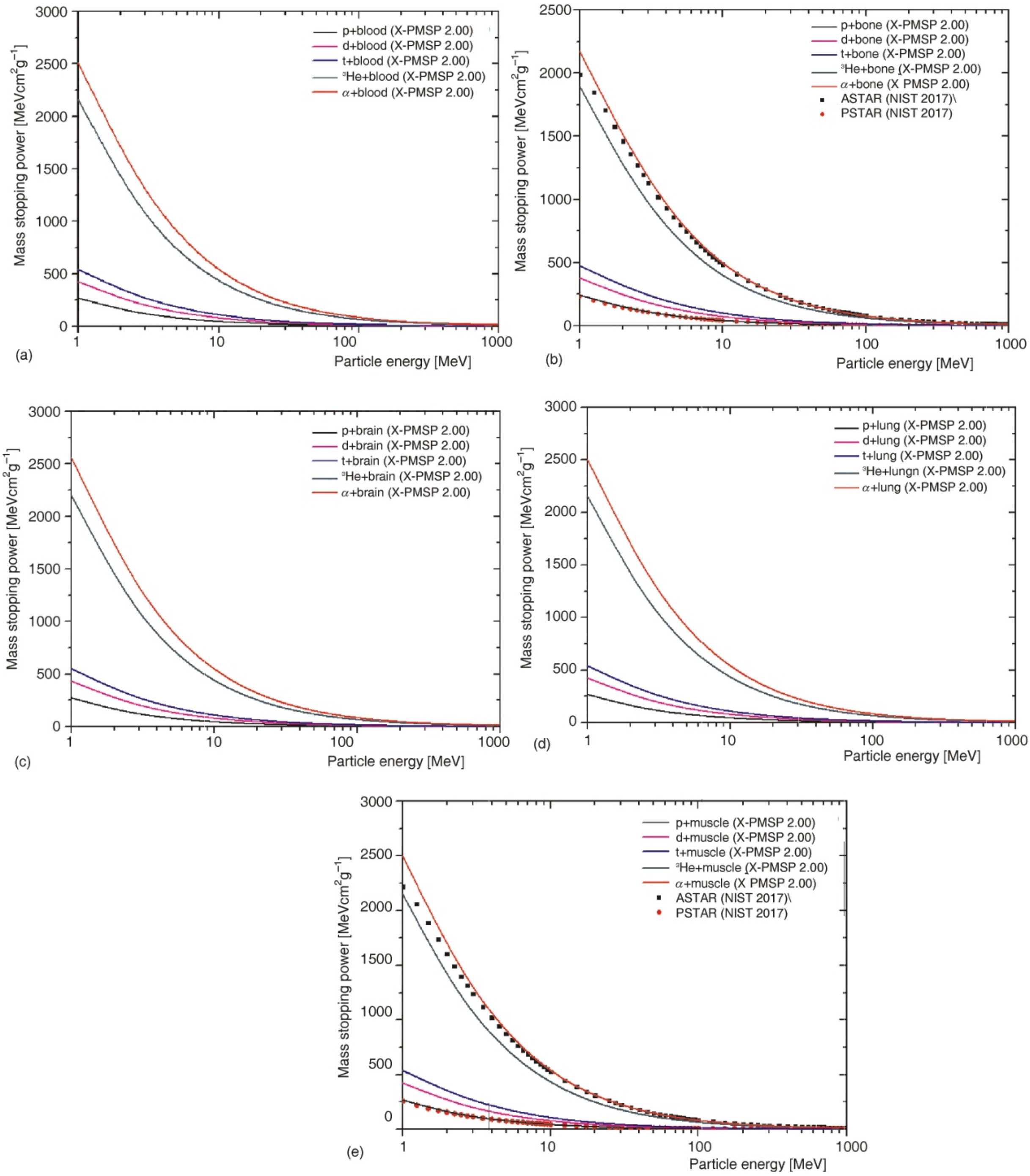

Figure 1. The mass stopping power calculations for proton, deuteron, triton, helium-3, and alpha particles on blood, bone, brain, lung and muscle

pha particles and at 1-250 MeV for protons, wherein the error rate is 10 %.

In addition to calculating the stopping powers of the available 180 compounds and mixtures in Sternheimer *et al*.'s [11] table, X-PMSP 2.0 can calculate the stopping powers of new compounds and mixtures defined by the user, based on their chemical formula alone. However, there can be some discrepancy in the stopping powers results obtained by the second and the third methods of the program. Because, the third method uses Paul and Schinner's [10] approach in calculating the mean excitation potential of the medium for materials I instead of Sternheimer *et al*.'s [11] table. To compare both approaches, a new section was added as follows.

Discussion of methods in X-PMSP

To understate the difference between the methods, we utilized the stopping powers of air (near sea level). In method 2, the density effect parameter and the mean excitation potential of the medium are obtained from the data reported by Sternheimer *et al*., [11]

Table 1. The error rates of mass stopping powers of some substances for proton particles

	Energy ranges for proton particles [MeV]						
Substances	1-5	5-10	10-50	1-100	1-250	1-500	1-1000
Bone	2.4197	0.4546	3.0911	4.6516	7.0851	10.8965	20.6785
Muscle	2.2425	0.3535	3.2289	4.6731	7.1174	10.8634	20.5691
Aluminum oxide [AlO]	3.2947	0.9512	2.8830	4.7618	7.1438	10.8586	20.6067
Glass. borosilicate (pyrex)	3.1896	0.8544	2.9282	4.7497	7.1395	10.7810	20.4758
Polyethylene	1.8108	0.3283	3.3593	4.6687	7.1312	13.6211	25.6344
Propane	1.5808	0.3434	3.3858	5.6725	8.1513	11.8872	21.4620
Air. (dry) for method 2	2.8278	0.4215	3.1674	4.7419	7.6890	11.7618	21.6378
Air. (dry) for method 3	0.6411	1.6783	4.6989	5.5534	8.0049	11.2216	20.4728

Table 2. The error rates of mass stopping powers of some substances for alpha particles

	Energy ranges for alpha particles [MeV]						
Substances	1-5	5-10	10-50	1-100	1-250	1-500	1-1000
Bone	4.6825	2.7971	0.8241	2.1203	2.6377	3.8181	7.0959
Muscle	6.4213	2.8974	0.7933	2.4427	2.9191	4.0673	7.3118
Aluminum oxide (AlO)	4.6319	3.2002	1.1039	2.1931	2.6733	3.8291	7.0665
Glass. borosilicate (pyrex)	4.9699	3.2316	1.0595	2.2484	2.7217	3.8730	7.1078
Polyethylene	5.9794	2.5951	0.7097	2.3446	2.8542	4.0247	7.2972
Propane	8.0366	2.3461	0.6814	2.6048	3.0727	4.2149	7.4625
Air. (dry) for method 2	6.3581	3.4915	0.8995	2.5521	3.0022	4.1325	7.3511
Air. (dry) for method 3	1.8833	0.6199	1.5015	2.1398	2.9167	4.2394	7.6254

whereas method 3 uses Paul and Schinner's [10] approach in eq. (2) for determining the mean excitation potential of the medium. Comparison of the two methods is presented in fig. 3. The ASTAR and PSTAR results in fig. 3 are in good agreement with those of both methods, however, in the energy region 1-20 MeV, stopping power results for alpha particles using method 3 were closer to the ASTAR data than those calculated using method 2, especially in the range 1-5 MeV. These results indicate that compared with the method 2, the calculation of stopping powers, based on the mean excitation potential of the medium, obtained from Paul and Schinner's approach (method 3) in compounds and mixtures, gives more accurate results with a small difference.

CONCLUSIONS

The knowledge of mass stopping powers of materials is essential in charged particle radiotherapy, radioisotope production for diagnostic (PET and SPECT) and therapeutics, radioisotope production for energy generation, and shielding of nuclear reactors and accelerators. Thus, we developed the X-PMSP 2.0 program to calculate the mass stopping powers of various medical, chemical, and industrial compounds and mixtures, such as blood, bones, lungs, brain, muscles, AlO, glass, polyethylene, propane, and air, for proton, deuteron, triton, helium-3 and alpha particles, and compared the obtained results with those from the NIST databases.

This comparison revealed that the calculated results of X-PMSP 2.0 are consistent with those of the NIST databases, which contain the most comprehensive data in the literature. However, there is a deficiency in the mass stopping power calculations for deuteron, triton and helium-3 charged particles, as well as proton and alpha particles. In particular, radioisotopes used in PET and SPECT can be also produced by deuteron, triton and helium-3 induced particles, in addition to those by proton and alpha particles, because the mass stopping power values are used for yield calculations. Therefore, the program overcomes the shortcomings in the literature. In the energy region 10-50 MeV, corresponding to the production energy of PET and SPECT radioisotopes, the error levels of the program were noted to be <5 % for protons and <2 % for alpha particles.

When taking into account the shielding of charged particles emitted during reactions in nuclear reactors and particle accelerators, determining the energy loss of charged particles inside the material is crucial, which is also facilitated by X-PMSP 2.0 program for the energy region 1-250 MeV for protons and 1-1000 MeV for alpha particles.

In charged particle radiotherapy of body tissues/organs (brain, lung, bone, *etc.*) with tumors, the mass stopping power calculation results for the charged particle using X-PMSP were found to be in good agreement with the data in the literature. Using this program, the stopping powers used in the calculations of penetration depths of ranges of different types of beams, can be determined for different human tissues and cancer cells, using just the formulation of substance prepared by the

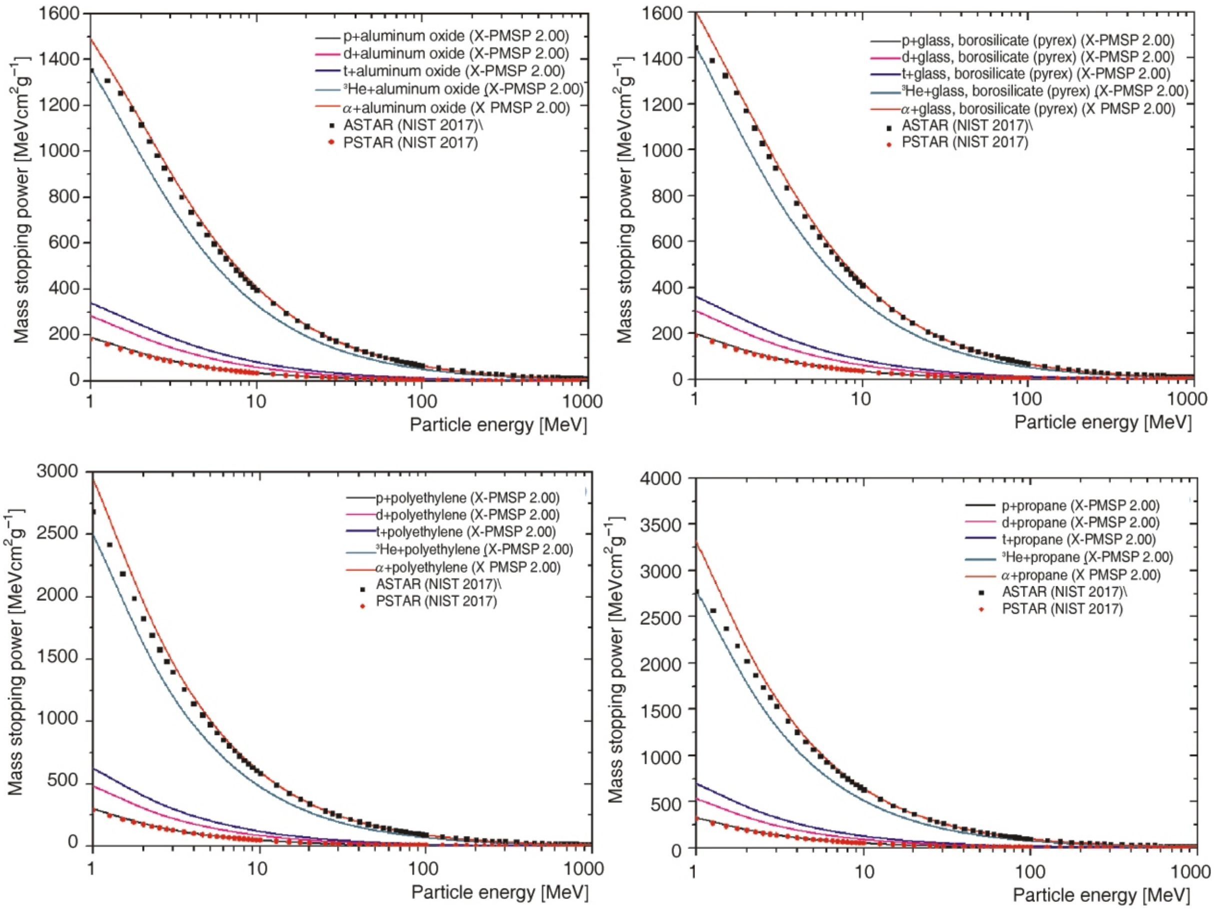

Figure 2. The mass stopping power calculations for proton, deuteron, triton, helium-3, and alpha particles on aluminum oxide, glass, polyethylene, propane

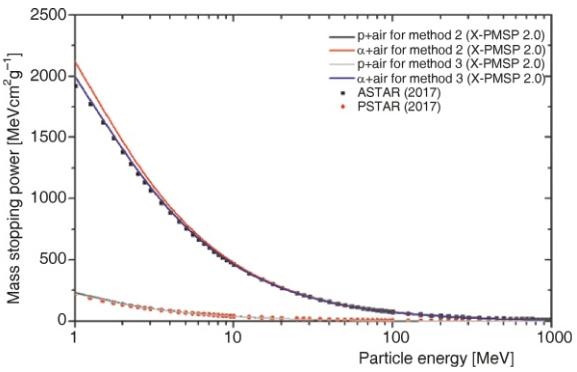

Figure 3. The comparison of method 2 and method 3 for proton, deuteron, triton, helium-3, and alpha mass stopping power calculations on air

user. The calculated results for the energy region 1-250 MeV, used in charged particle radiotherapy, have the maximum error rates of ~8.2 % for protons and of ~3.0 % for alpha particles. It is clearly explained that an experimenter may rely on this program, in charged particle radiotherapy.

Furthermore, the number of materials used in the present study is inadequate to debate the mass stopping powers results, especially for deuteron, triton and helium-3 particles. Therefore, both theoretical calculations and experimental results indicate that further detailed studies on the mass stopping power calculation for radiotherapy, radioisotope production, and shielding, are required to confirm the energy loss of charged particles, inside materials. Hence, future studies associated with the stopping power calculations should involve many substances, and related experiments using newer irradiation technologies, should be carried out. In line with the calculated results and the experimental data, we can recommend a semi-empirical stopping power formula for the next version of X-PMSP using artificial intelligence, such as fuzzy logic and artificial neural network.

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ПРОРАЧУН МАСЕНЕ ЗАУСТАВНЕ МОЋИ МЕДИЦИНСКИХ, ХЕМИЈСКИХ И ИНДУСТРИЈСКИХ ЈЕДИЊЕЊА И СМЕША

У овом раду развијена је нова верзија програмског пакета X-PMSP за процену масених зауставних моћи у радиотерапији наелектрисаним честицама, прорачуну заштите нуклеарних реактора, акцелераторима честица и производњи медицинских и енергетских радиоизотопа. Применом X-PMSP програмског пакета израчунали смо масене зауставне моћи важнијих медицинских, хемијских и индустријских једињена и смеша дефинисаних од стране Међународне комисије за радијационе јединице и мере у циљу доприноса постојећој литаратури и поређења наших резултата са подацима Националног института за стандарде и технологију. Примена овог програмског пакета, у опсегу енергија од 10 MeV до 50 MeV, биће значајна у области производње медицинских радиоизотопа јер смањује максималну стопу грешке испод 5 % за протоне и до 1.6 % за алфа честице. Додатно, максималне стопа грешака у радиотерапији наелектрисаним честицама, за опсеге од 1 MeV до 250 MeV, износе 8.2 % за протоне и 3.0 % за алфа честице.

Кључне речи: зауставна моћ, заштитини материјал, медицински материјал