A Comparative Study for the Proton Electronic Stopping Power of Some Polymers by Using Mathematica, SRIM2013, PSTAR, LibdEdx, and Experimental Databases

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Received in :10/April/2017،Accepted in :3/May/2017

Abstract

The available experimental data of proton electronic stopping power for Polyethylene, Mylar, Kapton and Polystyrene are compared with Mathematica, SRIM2013, PSTAR and libdEdx programs or databases. The comparison involves sketching out both experimental and databases data for each polymer to discuss the agreement. Further, we use statistical means via standard deviation resulting from the mean normalized difference to describe the precise agreement among the databases and the experimental data. We found that there is not a specific one database can describe the experimental data for certain material at given proton energy.

Keywords: Proton Electronic Stopping Power, Mathematica, SRIM2013, PSTAR, libdEdx, Polymers**.**

Introduction

Stopping power referred to the rate that charge particles lose energy in their travel through a certain material [1]. It consists of two parts, the Electronic Stopping Power (ESP) and Nuclear Stopping Power (NSP). The former results in due to the slowing down of ion and are attributed to interaction of incidence ions with the bound electrons of the material as a result of inelastic collisions. The last process expresses that the energy is lost by the ions that are dissipated out of electron cloud into thermal vibrations of the material. The collisions involved both excitations of electron cloud and bound electrons of the material [2].

There are several physical models that describe the (ESP) [3]. However, it is difficult to represent the entire interactions involved due to large number of collisions and the frequently change of ion charge state that traverse the material [4]. For example, the Bethe formula considers the (ESP) in high energy range as momentum transfer between ion and electrons of the target. Theoretically it is very difficult to determine the accurate (ESP) and thus various programs yield different (ESP) depending on the manner of calculations and considerations.

The programs used for our purpose are Mathematica, SRIM2013, PSTAR, and libdEdx. The Mathematica is a mathematical commercial software uses in many scientific fields. The newest version of Mathematica provides a database for stopping power for so many elements and materials at any given ion energy. The other well – known database is the SRIM2013, or Stopping and Range of Ions Matter, which calculates the interaction of ions with matter based on Monte Carlo simulation. This program provides tables for stopping power for ions and various materials. The other well – known database is the PSTAR, which calculates the stopping power and range for ions in many elements and 74 materials. The PSTAR database uses methods that are described in ICRU 37+49 reports [5]. The original libdEdx program is written in C which provides libraries to calculate variety of stopping power. However, the website dEdx provides a java script front end to the libdEdx stopping power library and for many additional libraries including libdEdx. We choose for our propose ICRU73+49 that is described in ICRU 73+49 reports and BETHE-EXT00 to collect the (ESP) from this website. The BETHE-EXT00 is working of Bethe equation expanded to low proton energy and is implemented as a function not based on tabulated data [6].

The plastics and polymers under investigation are Polyethylene $(CH_2CH_2)_n$ which is most common plastic material used in plastic bags and container such as bottles. The second material is the Polyethylene Terephthalate (Mylar) $(C_{10}H_8O_4)_n$ is a thermoplastic polymer resin of polyester used as a fiber for liquid and foods containers and as fibers for clothing. The third material used here is the Polyimide film $(C_{22}H_{10}N_2O_5)_n$ is a polymer known as a Kapton, which has high heat resistance and then uses various military applications. The last polymer is the Polystyrene $(C_6H_5CHCH_2)_n$, which is a synthetic aromatic polymer used as disposable cutlery and protective packaging such as DVD and CD cases.

The aim of this research is to test the agreement among experimental and databases for the (ESP) using some polymers by graphs and statistical means. Thus it can be decided which of these programs are closer to the experimental data and whether these programs are compatible with each other or mismatch. Due to lower effect of (NSP) on total stopping power, we involve with (ESP) only for our purpose.

Theory

To facilitate the calculations for the sake of statistical comparison, the experimental and databases data are casting to a specific range. The normalized difference between experimental and any set database is given by [7]

$$\delta = 100 \times \frac{(S_{\text{exp}} - S_{\text{table}})}{S_{\text{exp}}} \quad (1)$$

where S_{exp} , S_{table} are the experimental and table electronic stopping power, respectively. The mean normalized difference between experimental and any corresponding database is calculated for the same material and same proton energy [7]

$$\Delta = \langle \delta \rangle \quad (2)$$

then the standard deviation is calculated using [7]

$$\sigma = \sqrt{\langle \delta^2 \rangle - \langle \delta \rangle^2} \quad (3)$$

Results and discussion

The (ESPs) of the Polyethylene are shown in Figure (1) for both databases used and the three available of experimental data. The (ESP) increases rapidly with increasing energy of protons reaching to a maximum and then slowly decreases. One can divide roughly the curves of (ESP) into three categories by energy of the incidence proton; low where the curves are raising, intermediate where the maximums of (ESP) occur, and high where the curves have decreasing exponential behavior. At the low and intermediate proton energy the SRIM2013 calculations indicate higher (ESP) than the other counterparts programs, while this curve is less than the rest of the programs in the high proton energy. The Mathematica, PSTAR and libdedx (ICRU73+49) give approximately similar results. On the other hand the libdEdx (BETHE-EXT00) gives lower curve in the low and intermediate regions but not in the higher energy. The curves of Mathematica, PSTAR and libdedx (ICRU73+49) databases are lower than SRIM2013 curve in low and intermediate regions of energy, while it is higher than the SRIM2013 curve at high proton energy. It is clear that the peak of the (ESP) for SRIM2013 database is higher in value than the other programs. Further, it is shifted to the left compared to the other peaks of databases. It is noted that the peak for libdEdx (BETHE-EXT00) is located at relatively higher proton energy. At higher proton energies, the entire databases relatively match the calculations of each other. It notes that for the experimental data (Refs 8-10) are relatively described by the PSTAR, libdEdx (ICRU49-73) and Mathematica databases. Only few points of Ref. (10) data are lying on SRIM2013 database and it is far from the other program curves. In respect to data of Ref (9), only some points are nearly lying on SRIM2013 curve that are closed to the maximum.

Similar to Polyethylene Figure (2) shows the (ESP) as a function of proton energy for Mylar. Clearly various databases yield different values of the (ESP) in low and intermediate proton energies, however, the curves are close to each other at the high energy used. The maximum of the (ESP) for libdEdx (BETHE-EXT00) database is shifted to the higher proton energy compared with the rest of the databases and this curve is lower than the curves of other programs. The Mathematica, PSTAR, and libdEdx (ICRU49+73) databases are identical since the curves match on each other. The curves of (ESP) as a function of proton energy for Mylar continue to mismatch as the proton energy increased and finally match on another at the high proton energies for SRIM2013, libdEdx (BETHE-EXT00) databases. The experimental data for Mylar are limited to a high energy region for the energy range used. The data of Ref. (11) above 2 MeV agree with the all the databases used. But at higher than this energy, they dispersed between compatibility and incompatibility. All the points of Ref. (12) are located on the curves of programs, while the Ref. data (13) are relatively coincide with curves of Mathematica, PSTAR, and libdEdx (ICRU49+73) databases. Regarding to the data of Ref. (14) most of points are placed lower than the curves of these three databases compared with the ref. data (15) where the points are located on these curves. The libdEdx (BETHE-EXT00) database is well to describe the data of Ref. (16). The agreement between experimental data and the using databases would be clear on our discussion with statistical tools

Figure (3) shows the variations of (ESP) verses proton energy using the entire databases used with the available experimental data for the Kapton. Obviously, the libdEdx (BETHE-EXT00) database gives a curve that shift to the right towards the higher proton energies compared to curves of the rest of the databases. This shift is lying at the intermediate

energy domain. At highest energies all the databases curves are compatible. Further the peak of (ESP) curve for the libdEdx (BETHE-EXT00) database is lower compared to the other databases peaks. At the beginning of increased proton energy, the curve of (ESP) due to SRIM2013 database is lower than the other rest three databases expect libdEdx (BETHE-EXT00). The curves of the four databases then meet at the proton energy equal to 0.037 MeV. After this energy the curve of (ESP) for the SRIM2013 is lower than other three databases. The curves continue to rise but the curve peak of SRIM2013 is less than that of other three databases. All (ESPs) of entire databases meet at proton energy of 160.4 MeV.

The calculations of (ESP) in Polystyrene are shown in Figure (4). For the Polystyrene the entire databases except libdEdx (BETHE-EXT00) and SRIM2013 still give identical curves of (ESP). It is noted that for all the polymers used the curve of (ESPs) in libdEdx (BETHE-EXT00) database is lower than the curves of the rest of the databases. Again the maximum of the (ESP) curve in the libdEdx (BETHE-EXT00) database is shifted to the right towards the high energies, in the intermediate proton energy range. At higher proton energies the differences in calculations are relatively very little and the decreasing of the differences soon is very small at higher protons since all curves match each other.

Figure (5) shows (ESP) of the databases for all polymers used. The databases share the same behavior the (ESP). The differences of (ESP) for the polymers used depend on it chemical structure. Obviously, the Polyethylene has a higher (ESP) compared to the other polymers. It is interesting that the Mylar and Kapton curves coincide on each other due to SRIM2013 calculations. Moreover, Figure (5) shows the matching of curves for Mathematica, PSTAR, and libdEdx (ICRU49+73) databases. Generally the libdEdx (BETHE-EXT00) gives lower curves for the polymers compared to other databases.

Statistically to describe the agreement between two sets of data, one could use the standard deviation σ resulting from means normalized difference Δ of experimental and databases data. For this purpose, we build a Matlab program to achieve the calculations and explain the agreement. Tables (1) show Δ and its σ calculations between experimental and mentioned databases data for the used polymers. Normally, the difference of two means denotes the range where these values may lie. It specifies the confidence interval for these differences. This statistical tool gives interesting information to compare two data parameters. For a given level of confidence, it may consist zero and in this case the difference of two means has no any significant. The standard deviation σ denotes how far the data are spread below and above the Δ. This means that a high σ gives a widely spread of the data around Δ or less reliable results. On the other side the more reliable results are to have low σ where the data are collected closely around Δ. The perfect or high agreement between two data is when the σ equals to zero. Thus the smaller σ is the narrower range between both the experimental and theoretical data.

For Polyethylene, in the given restricted range, the database ICRU49+37 is the best to describe experimental data of Ref (8 and 9) compared to other databases due to smaller σ. The σ gives the accuracy of database table and signifies the best agreement between experimental and this database table. The PSTAR table yields good agreement with experimental data of Ref (10) due to lower σ . Since Δ and σ of the libdEdx (BETHE-EXT00) are larger than other databases, so it is far away from agreement with experimental data.

There are six references of experimental data for Mylar. However, we cannot decide the good agreement of all those with the mentioned databases. The Mathematica is characterized by its ability to calculate the (ESP) by any fraction of protons energy for given material, but unfortunately, other databases cannot. Therefore, we cannot decide the good agreement for all those experimental data expect for Refs (12, 13). Mathematica database describes good agreement with data of Ref (12) for Mylar, and PSTAR with Ref (13) have lower σ compared to other databases, thus well agreement between experimental data and this database is obtained.

For the same reason mentioned above, we give the calculations of Mathematica only since the data of Refs. (17 – 19) for Kapton are not supported by the rest of databases used. Here, we cannot decide the agreement priority of database over others.

Finally, for Polystyrene the SRIM2013 database has a better agreement compared to the programs for data of Refs (21, 2, 3), while PSTAR achieved good agreement with data of Ref (1).

Conclusion and Suggestion

The (ESP) data for certain polymer is different for various databases. The (ESP) data for given database depends on manner of calculations and the parameters involved. One cannot decide the good agreement among those databases and experimental data by sketching out the diagrams only. By using the statistical tools, we can examine how far the agreement between the database and experimental data are approaching the reality. With this sense, we suggest using other statistical means to examine the agreement between empirical data and programs such as Chi square goodness of fit test.

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Tables (1) describe the experimental data as a reference compared with used programs (a –p).

Polyethylene	Ref. (8)		Ref. (9)	Ref. (10)
Energy (MeV)	0.4 − 0.1		0.032 − 0.335	0.04 – 0.35
No. of Points	13		19	17
Mathematica	Δ	−0.6062	4.1789	−0.2071
	σ	±1.7764	±1.0408	±0.8626

(a)

Polyethylene	Ref. (8)		Ref. (9)	Ref. (10)
Energy (MeV)	0.4 − 0.1		0.032 − 0.325	0.04 – 0.35
No. of Points	11		18	15
SRIM2013	Δ	2.2483	3.5271	−0.2501
	σ	±2.6466	±3.2685	±2.8319

(b)

Polyethylene	Ref. (8)		Ref. (9)	Ref. (10)
Energy (MeV)	0.4 − 0.1		0.032 − 0.335	0.04 – 0.35
No. of Points	13		19	17
PSTAR	Δ	−0.6399	4.1126	0.0373
	σ	±1.4428	±0.8598	±0.8393

(c)

Polyethylene	Ref. (8)		Ref. (9)	Ref. (10)
Energy (MeV)	0.4 − 0.1		0.032 − 0.325	0.04 – 0.35
No. of Points	10		18	15
ICRU49+73	Δ	0.0741	4.2892	0.0288
	σ	±1.2865	±0.9372	±0.8594

(d)

Polyethylene	Ref. (8)		Ref. (9)	Ref. (10)
Energy (MeV)	0.4 − 0.1		0.032 − 0.325	0.04 – 0.35
No. of Points	11		18	15
BETHE-EXT00	Δ	0.7056	9.7697	5.1949
	σ	±2.0641	±4.5753	±5.8839

(e)

Mylar	Ref. (11)		Ref. (12)	Ref. (13)	Ref. (14)	Ref. (15)	Ref. (16)
Energy(MeV)	0.336-8.26		4-11.5	0.4-3.25	0.289-1.942	0.2368-3.0196	1.091-3.502
No. of Points	39		16	17	17	35	11
Mathematica	Δ	−0.4843	−0.3340	0.3926	−2.0815	0.3586	5.1011
	σ	±3.1675	±0.1073	±0.6194	±1.2082	±0.6296	±1.6241

(f)

Mylar	Ref. (12)		Ref. (13)
Energy(MeV)	4- 11		0.4-3.25
No. of Points	11		14
SRIM	Δ	-2.0950	1.8297
	σ	± 0.1698	± 4.5624

(g)

Mylar	Ref. (12)		Ref. (13)
Energy(MeV)	4- 10		0.4-3
No. of Points	13		16
PSTAR	Δ	-0.3230	0.4404
	σ	± 0.1162	± 0.6065

(h)

Mylar	Ref. (12)		Ref. (13)
Energy(MeV)	4- 11		0.4-3.25
No. of Points	11		14
ICRU49+73	Δ	-0.3001	0.3878
	σ	± 0.1116	± 0.6625

(i)

Mylar	Ref. (12)		Ref. (13)
Energy(MeV)	4-11		0.4-3.25
No. of Points	11		14
BETHE_EXT00	Δ	-1.4717	-2.9953
	σ	± 0.3155	± 0.7910

(j)

Kapton	Ref. (17)		Ref. (18)	Ref. (19)
Energy(MeV)	0.5621- 1.5485		2.93- 8.28	0.857- 2.93
No. of Points	39		23	9
Mathematica	Δ	0.6293	-5.0201	2.6476
	σ	± 0.7820	± 2.2790	± 2.3830

(k)

Polystyrene	Ref. (20)		Ref. (21)	Ref. (22)	Ref. (1)	Ref. (23)	Ref. (24)	Ref. (2)	Ref. (25)	Ref. (3)
Energy (MeV)	0.899 - 2.966		0.04- 0.4	2.248- 5.88	0.4- 0.1	0.1289- 0.4641	0.0699- 0.4882	0.025- 0.335	0.0325- 0.9069	0.04- 0.35
No. of Points	9		16	13	13	18	25	20	12	17
Mathematica	Δ	3.5586	0.2623	-0.1008	1.7017	5.8543	5.6708	4.3267	3.0050	3.7824
	σ	± 2.2292	± 7.5523	± 0.5909	± 0.8044	± 2.1728	± 3.0814	± 3.3457	± 5.5025	± 2.6314

(l)

Polystyrene	Ref. (21)		Ref. (1)	Ref. (2)	Ref. (3)
Energy (MeV)	0.04-0.4		0.4-0.1	0.025-0.325	0.04-0.35
No. of Points	12		11	19	15
SRIM2013	Δ	-2.5783	-1.5895	3.8732	2.7438
	σ	± 4.9696	± 0.8580	± 1.2664	± 0.9403

(m)

Polystyrene	Ref. (21)		Ref. (1)	Ref. (2)	Ref. (3)
Energy (MeV)	0.04-0.4		0.4-0.1	0.025-0.3	0.04-0.35
No. of Points	8		11	14	16
PSTAR	Δ	-3.5537	1.8343	3.2750	3.7598
	σ	± 9.0713	± 0.7804	± 3.4592	± 2.7110

(n)

Polystyrene	Ref. (21)		Ref. (1)	Ref. (2)	Ref. (3)
Energy (MeV)	0.04-0.4		0.4-0.1	0.025-0.325	0.04-0.35
No. of Points	12		11	19	15
ICRU49+73	Δ	-1.2944	1.5757	4.2510	3.6600
	σ	± 8.0147	± 0.7992	± 3.4078	± 2.7740

(o)

Polystyrene	Ref. (21)		Ref. (1)	Ref. (2)	Ref. (3)
Energy (MeV)	0.04-0.4		0.4-0.1	0.025-0.325	0.04-0.35
No. of Points	12		11	19	15
BETHE-EXT00	Δ	7.6009	0.3918	16.7056	13.3676
	σ	± 8.0845	± 6.0107	± 11.8123	± 11.5840

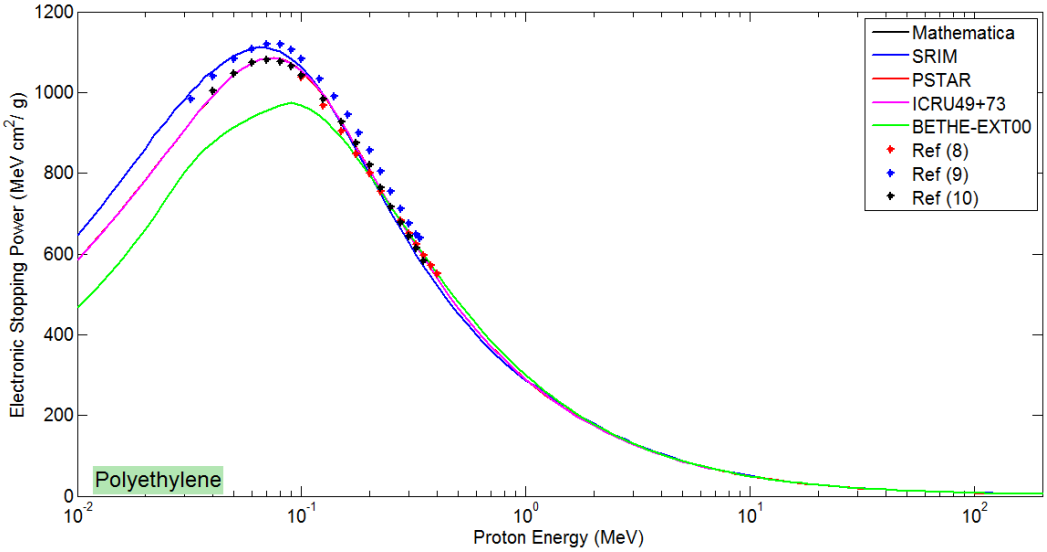

Figure (1): The electronic stopping power verses proton energy for Polyethylene for some databases used and available experimental data.

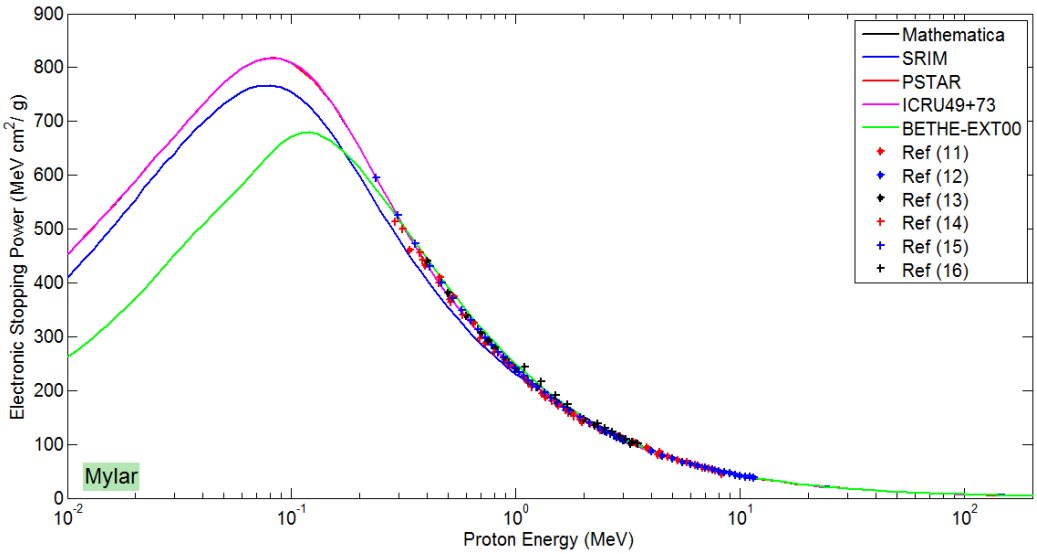

Figure (2): The electronic stopping power for Mylar as a function of protons energy for the databases used and for some available experimental data.

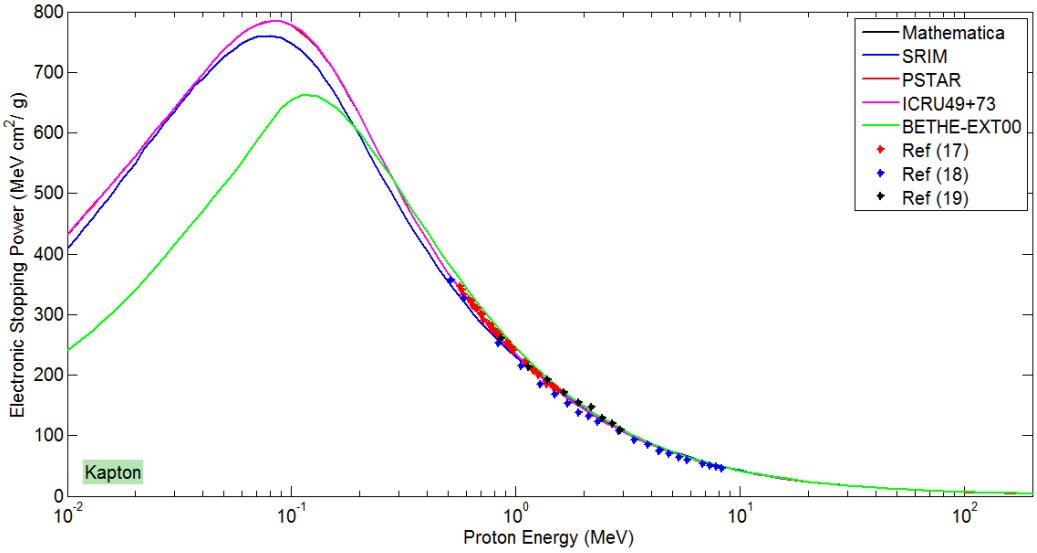

Figure (3): The electronic stopping power as a function of proton energy calculated by using different programs and the experimental data for Kapton.

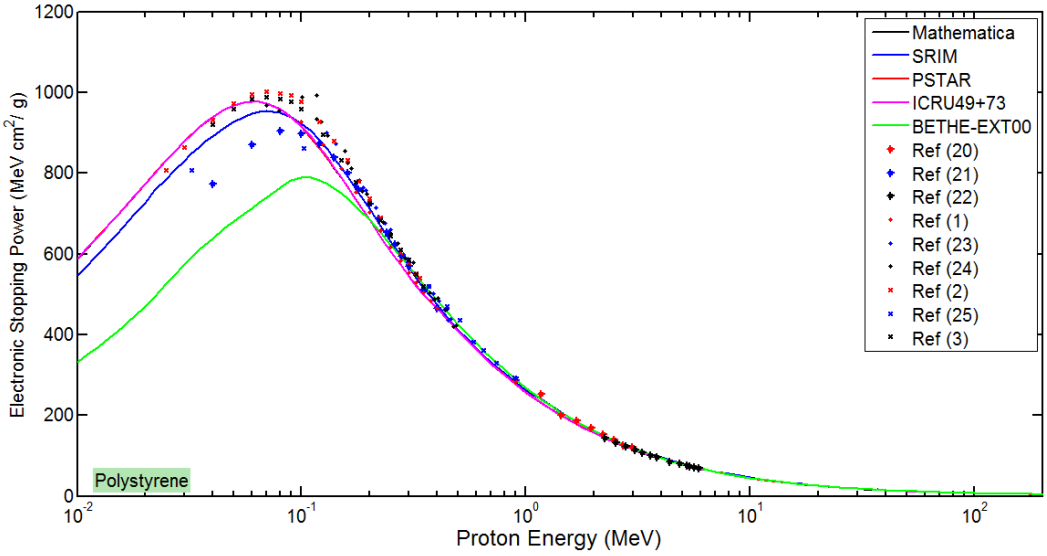

Figure (4): The electronic stopping power verses proton energy for Polystyrene for some programs used and available experimental data.

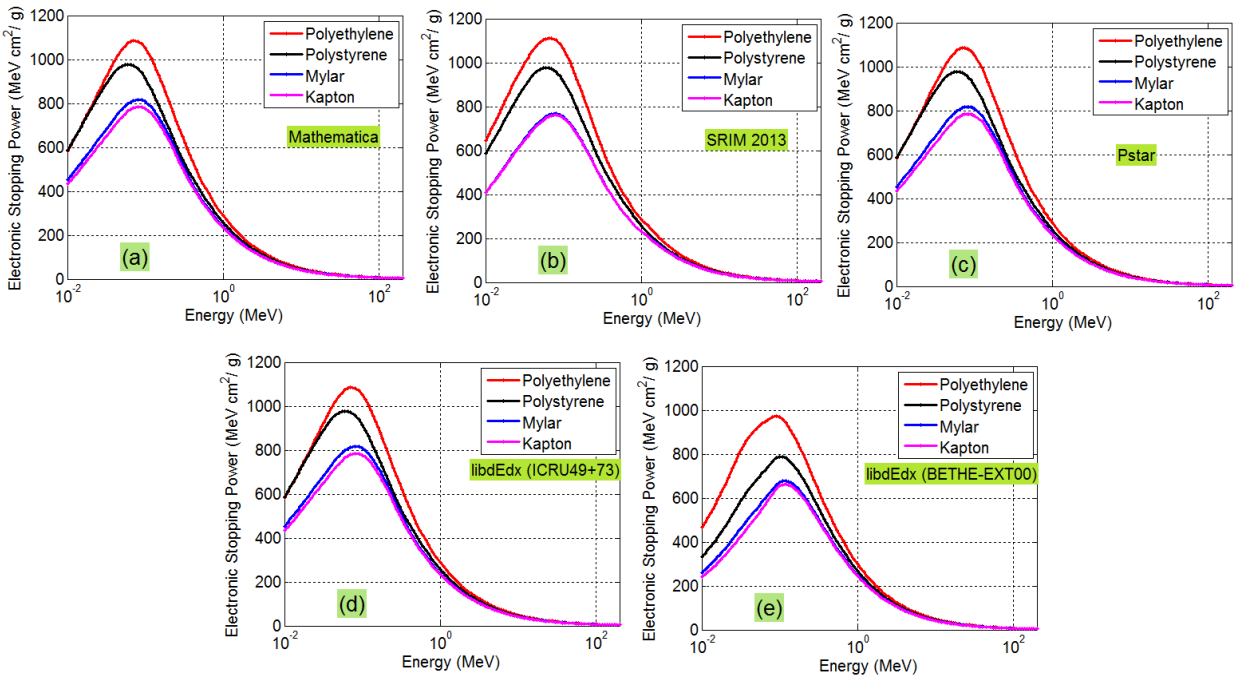

Figure (5): The electronic stopping power as a function of proton energy calculated for different polymers by using (a) Mathematica (b) SRIM2013 2013 (c) PSTAR (d) libdEdx (ICRU49+73) (e) libdEdx (BETHE-EXT00).