Advances in Physics Theories and Applications ISSN 2224-719X (Paper) ISSN 2225-0638 (Online) Vol.66, 2017



Statistical Investigations on the Extent of Convergence or Divergence of Some Electronic Stopping Power Programs with Experimental Data

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Abstract

A comparative comparison among the experimental electronic stopping power with some common program data for proton, Helium, and Boron ions with different targets are graphically achieved. For certain specific energy ranges the impact of various programs is investigated by using two statistical tests. The tests are Chi square goodness of fit and standard deviation computed from the mean normalized difference. It is found that for the certain ion-target combinations, these programs with its different data given are relatively close or far away to match the experimental data. By using those tests for ion-target combinations we determine within given accuracy the best agreement among programs and experimental data.

Keywords: Electronic Stopping Power databases, proton, Helium ion, Boron ion, Chi square of goodness of fit test, standard deviation test.

1. Introduction

It is known that the ions undergo to a series of collisions within a target material as it travel inside the target until finally come to rest at a certain depth. The whole process is typically losing the energy by two mechanisms: nuclear and electronic stopping (Backman 2012). The former is responsible for the damage of target material and lattice disorder due to transfer of ion energy to target by elastic collision. The electronic stopping is caused by the interaction of ions with the target bound electrons. This process is inelastic and the ion energy is dissipated over the cloud of electron to target thermal vibrations. Thus, the stopping power is ions lose energy as it travels through the material (Giannuzzi et al. 2005). The Total Stopping Power (TSP) is then the addition of Nuclear Stopping Power (NSP) and Electronic Stopping Power (ESP). The importance of these two processes is relatively dependent on the ion energy and its atomic number. On the other hand, the nuclear collisions are dominated at low ion energy and the electron collisions take control at the high ions energy (Möller 2004). It seems difficult to represent the entire processes involved in the interactions between ion and the material. Therefore, there are many mathematical models to describe the interactions because of the large number of collisions and changing the ion charge state that can be included (Tavernier 2010). There are huge benefits to search on a topic of interaction of the charged particles with matter, especially ion therapy of medical physics where the range of penetration is derived in the slowing down approximation (Jafer 2009 & U.S Dept. of Energy 2013). We in this paper for the purpose of this work do not treat NSP, nor TSP, but ESP due to the somehow large experimental data availability of it.

There are several programs are available to provide the ESP of ions – target combinations with different applicable range. The ESP can be implemented using programs such as SRIM, ASTAR, MSTAR, PSTAR, ICRU49+73, BETHE-EXT00, and recently MATHEMATICA. SRIM (Stopping and Range of Ions in Matter) is a program provides databases for, various ion-target combinations through quantum mechanical treatment of ion - atom collisions (Ziegler 2013). The NIST (National Institute of Standards and Technology) supplies the databases PSTAR and ASTAR that calculate ESP for protons and helium ions, respectively, according to some methods described in ICRU Reports 37 and 49 (Berger *et al.* 2005). MSTAR calculates ESP contained in ICRU Reports 49 that is based upon ⁴He and then extended for heavy ions. The heavier ions that can implement in MSTAR are not covered by ASTAR and PSTAR (Paul 2004). The software libdEdx provides easy entrance to calculate ESP data, but it is available for Linux users (libdEdx). However, the dEdx website provides a Java script front end to the libdEdx ESP library. The dEdx is inspired by PSTAR, ASTAR and additional libraries such as BETHE-EXT00 (Bethe-equation expanded to low energy) and ICRU49+73 for so much material compositions (Toftegaard *et al.* 2014). Generally, various programs produce different ESP, depending on theoretical or empirical considerations or algorithm involved in the calculations and therefore there are often deviation among them in the magnitude for certain ion, target and energy. We use these programs to calculate ESP as a function of protons, ⁴He, and Boron for alternative different

We use these programs to calculate ESP as a function of protons, ⁴He, and Boron for alternative different target material like solids or gases for sake of comparison among these programs and experimental data results. The comparisons are carried out by sketching graphs of experimental and programs data and using two statistical means to denote whether there is significant difference between the programs and among them with experimental data. By this way we can by a careful sight, relying on the experimental data, to determine which relevant program data are approaching or moving away from it for the specific combinations of ion- target and

the ion energy.

2. The statistical tests

The reliability of experimental and programs data (or databases) can be determined by the means of statistical comparisons. We choose differently two tests on their bases for this purpose. The first is the Chi square goodness of fit test and the second is the standard deviation computed from the mean normalized difference. The first test is a function that locates whether the categorized observed sample of data can be looked to match the categorized expected sample data, while the second determines by the standard deviation number how the spread of two data are.

2.1. Chi square goodness of fit test

To find out the assessment of whether the observed data can be claimed to reasonably fit the expected data for a given phenomenon, it often usually to use the Chi square goodness of fit test. It determines whether the observed data match the theoretical model (Kanji 2006). In this test the distributions of the observed sample and the expected probability are compared to denote the goodness of fit. The points of experimental data in a given range are compared with those points of each program in the same range interval for the same target and incident ion. Two hypotheses are involved in the test; null and alternative (Sheskin 2004). The null hypothesis postulates that there is no respectable variation between experimental and program data. The null hypothesis is rejected and gives a significant difference between experimental and calculated frequency whenever the value of Chi square goodness of fit is greater than critical program value. On the other hand, if the value of Chi square goodness of fit test is less than the critical program value, then there is no significant difference between them and the null hypothesis cannot be rejected. Since p-value is a probability, thus it is a real number from zero and one. Particulars, p-values are another way of measuring this. The p-value calculated in this test helps to reject or support the null hypothesis. The very large p-value signifies that the null hypothesis should not be rejected. On the other side, very small p-value causes to reject the hypothesis (Agarwal 2006).

2.2. The standard deviation test

For the purpose of statistical comparison, the calculations of both the experimental and programs data are casting to a specific range according to first data. For every point in the given specific ion energy, the normalized difference between experimental and any data of programs is

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

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where S_{exp} , S_{table} are the experimental and program electronic stopping power, respectively. For the certain material and certain ion energy the mean normalized difference between experimental and any corresponding program data is calculated and thus the standard deviation is calculated by (Stewart 2002)

$$\sigma = \sqrt{\langle \delta^2 \rangle - \langle \delta \rangle^2} \tag{2}$$

where the symbol () denotes an average.

The large standard deviation means that the data have spread. It is relative whether to consider a standard deviation to be small or not, but the smaller standard deviation always means that data is less spread out than larger.

3. Results and discussion

Figure (1a) shows ESP of Acetylene versus proton energy for one of available experimental data (Park & Zimmerman 1963) and some used programs. In low proton energy the ESP increases up to a peak in the intermediate proton energy region and then decreased exponentially at high energy. Clearly, various programs produce different results at lower proton energy. While the SRIM introduces a higher curve compared to other programs, the dEdx (BETHE-EXT00) gives lowest curve. The program's results even give locally different peak. In spite of that the calculations of entire programs match each other at relatively higher proton energies. The experimental data is located in small restricted range within the peak region. The data points shown in the tables indicate the size of how many experimental and programs points that have the same ion energy value as input in the statistical tests. For our purpose to introduce the agreement between experimental data and the programs used we use the mentioned two different tests; Chi square goodness of fit test function and standard deviation computed from the mean normalized difference. Table (I) summarizes the results of the first test for Acetylene bombarded by protons, while Table (II) expresses the results of another test for same ion-target combination. The first test results were implemented in Maple18 software package, whilst the other test is carried out by a small program in Matlab. The null hypothesis in in Chi square test for goodness of fit states that the observed sample does not differ from expected sample, while the alternative hypothesis says that the observed sample differs from expected sample. From Table (I) the only accepted null hypothesis is for SRIM whilst for other programs is rejected within the level of significance indicated. This is because the computed statistic is less than

 χ^2 value, respect to other programs. Moreover, the p-values for all the programs are zero except the SRIM where its p-value is positive number higher than zero. Therefore, the statement that the SRIM data is close to match the experimental data distribution is exactly justified. This conclusion is confirmed by the other statistical test achieved by standard deviation. The SRIM has the lowest value of standard deviation σ in table (II) among other. The smallest value of the SRIM standard deviation means the spread of the data around the mean difference are indeed low. The data are collected nearly close around the mean difference and this is the high reliable result to declare the best agreement of the SRIM. On the other side, the program BETHE-EXT00 has a larger value of computing statistic, which leads to more difference according to the computed critical value. Thus, this program is not approved among the programs used to express to goodness of fit. Again, this result is demonstrated by σ test. Table (II) shows highest σ for this program compared to other programs. This can be attributed to relatively wider of the spread of the data around the mean difference. As a result the BETHE-EXT00 is worse to express the agreement and far from accuracy respect to the experimental data.

Figure (1b) is a plot of ESP versus proton energy of Ethylene for the experimental (Park & Zimmerman 1963) and programs data. Similar mentioned behavior of ESP with proton energy as in Acetylene can be noticed. However, for this material the PSTAR-dEdx program gives a higher curve at the entire range of proton energy in comparison to other programs. It is noticed that the result of PSTAR-dEdx is slightly different from PSTAR-NIST database. The curves of them are not locally coinciding with each other due to different output resulting for the same energy and ion- target combination. For our objective with statistical comparison, Tables (III -IV) summarizes the results of both tests for proton-Ethylene. Tables (III) indicates again accepted the null hypothesis only for the SRIM respect to other programs. Obviously, there are two positive numbers of p-value for the SRIM and ICRU49+37. However, SRIM has accepted the null hypothesis but for ICRU49+37 is rejected. As mentioned above, the computed statistic value is smaller than χ^2 value for the SRIM leading to acceptance of the null hypothesis. On the other hand, the computed statistic value for ICRU49+37 is larger than χ^2 value and then the hypothesis is rejected even it has a small p-value but it is insignificant. Therefore, the SRIM is distributed with experimental data has the best goodness of fit. The second test would give the best program data that give the best agreement with experimental results. A glance to Table (IV) shows that the PSTAR-dEdx has smallest σ than other programs. The second program that has a good agreement is the SRIM due to the small σ value that ranked among the programs. The Table is assigned a bad agreement for the BETHE-EXT00 for its relatively higher standard deviation. Typically the first test describes the goodness of fit, measures the discrepancy between experimental and programs data that are dragged from identical distributions. The standard deviation test expresses the dispersal of points above and down the normalized mean difference. It gives comparative information between two data within the level of confidence. In other words, the PSTAR-dEdx data, due to its smaller σ , are clustered closely about the mean and then more reliable to specify the good agreement.



Figure (1): Electronic stopping power verses proton energy for (a) Acetylene (b) Ethylene for used programs and some of available experimental data (Park & Zimmerman 1963)

Table (I): Chi-Square Test for Goodness-of-Fit at level 0.05 for the experimental data (Park & Zimmerman 1963) with different programs for proton bombarded Acetylene.

Program	Hypothesis	Categories	Chi Squared	Distribution	P - value	Statistic
SRIM	True	11	18.307038053275	ChiSquared10	0.216868	13.1232
PSTAR - NIST	False	13	21.026069817483	ChiSquared12	0	185.61
PSTAR - libdEx	False	13	21.026069817483	ChiSquared12	0	185.502
ICRU49+73	False	13	21.026069817483	ChiSquared12	0	182.631
BETHE_EXT00	False	12	19.675137582166	ChiSquared11	0	443.352

Table (II): Standard deviation (STD) and mean normalized difference test for the experimental data (Park & Zimmerman 1963) with different programs for Acetylene bombarded by protons.

Program	SRIM	PSTAR - NIST	PSTAR - dEx	ICRU49+73	BETHE EXT00
Energy MeV	0.04 - 0.25	0.04 - 0.25	0.04 - 0.25	0.04 - 0.25	0.04 - 0.25
No. of points	11	13	13	13	12
Δ	0.9912	9.8600	9.8531	9.3061	13.5809
σ	±3.4755	±4.7028	±4.7049	±5.5729	±9.5307

 Table (III): Chi-Square Test for Goodness-of-Fit at level 0.05 for the experimental data (Park & Zimmerman 1963) with different programs for proton bombarded Ethylene.

Program	Hypothesis	Categories	Chi Squared	Distribution	P - value	Statistic
SRIM	True	11	18.307038053275	ChiSquared10	0.0719926	17.1087
PSTAR - NIST	False	13	21.026069817483	ChiSquared12	0	107.465
PSTAR - libdEx	False	13	21.026069817483	ChiSquared12	0	115.208
ICRU49+73	False	13	21.026069817483	ChiSquared12	0.0207349	23.9387
BETHE EXT00	False	12	21.026069817483	ChiSquared12	0	140.642

 Table (IV): Standard deviation (STD) and mean normalized difference test for the experimental data (Park & Zimmerman 1963) with different programs for Ethylene bombarded by protons.

SRIM	PSTAR - NIST	PSTAR - dEdx	ICRU49+73	BETHE_EXT00
0.04 - 0.25	0.04 - 0.25	0.04 - 0.25	0.04 - 0.25	0.04 - 0.25
11	13	13	13	12
-3.7481	3.8860	-9.5076	3.7977	8.0834
± 1.0832	± 1.1598	± 0.8768	± 1.1390	± 4.3233
	SRIM 0.04 - 0.25 11 -3.7481 ± 1.0832	SRIM PSTAR - NIST 0.04 - 0.25 0.04 - 0.25 11 13 -3.7481 3.8860 ± 1.0832 ± 1.1598	SRIM PSTAR - NIST PSTAR - dEdx 0.04 - 0.25 0.04 - 0.25 0.04 - 0.25 11 13 13 -3.7481 3.8860 -9.5076 ± 1.0832 ± 1.1598 ± 0.8768	SRIM PSTAR - NIST PSTAR - dEdx ICRU49+73 0.04 - 0.25 0.04 - 0.25 0.04 - 0.25 0.04 - 0.25 11 13 13 13 -3.7481 3.8860 -9.5076 3.7977 ± 1.0832 ± 1.1598 ± 0.8768 ± 1.1390

Figure (2a) expresses the variation of ESP verses Helium ion energy using the mentioned programs as well as MSATR and only for one of the available experimental data (Santry & Werner 1986) for the Aluminum Oxide. It should be noted that the program MSTAR gives same results when implemented directly using DOS version or from dEdx program. So, all MSTAR's calculations in this work were limited to the results of dEdx database. Obviously from the figure (2a), the SRIM gives a curve higher than the experimental data. The experimental data are excellently matching the curve of ASTAR-NIST database. The curves of ASTAR-dEdx, ICRU49-73, and MSTAR programs are in perfect matching on each other but not with experimental data. It shifted to the left from the experimental data towards lower energies. The curve of last program (BETHE-EXT00) is also shifted to the same energy region, but has lower values of ESP with ions energy. After the intermediate energy domain, the curve of BETHE-EXT00 program coincides exactly with the curves of the last mentioned three programs. In order to observe the goodness of fit among experimental and programs data, Table (V) expresses the true hypothesis for the ASTAR-NIST with somehow low p-value. The other programs rejected the null hypothesis and then have a badness of fit. The better goodness of program fit with experimental data is with any program with specific p-value and true hypothesis. Clearly, the computed statistics for the SRIM is lower than the other corresponding programs, but not for ASTAR-NIST. Further, the Chi distribution function of SRIM is different with a higher order. The difference between the computed statistics and the critical value is relatively smaller than other programs. This would affect the good agreement achieved with the second test. Table (VI) shows that ASTAR-NIST has a smaller σ compared to other programs. SRIM follows ASTAR-NIST in terms of small standard deviation value. Thus, the best agreement of experimental with program data is for ASTAR-NIST followed by SRIM.

Figure (2b) shows (ESP) of the programs and experimental data (Bourland *et al.* 1971) for Carbon Dioxide gas as a function of Helium ion energy. All programs have a similar behavior as in Figure (2a) for the Aluminum Oxide. The experimental data apparently very close to lie down on the curve of ESP vs. ion energy for SRIM and ASTAR-NIST programs. The other remaining program's curve needs to be shifted to right towards higher energy to conform higher matching to experimental data. The outline of this debate is confirmed by statistical

means. Table (VII) shows the results of the Chi square test for goodness of fit. It elucidates that ASTAR-NIST program has a relatively big p-value. Therefore, this gives a true statement to the null hypothesis. Further, it confirmed by the χ^2 value which is larger than the computed statistic. Since the null hypothesis is accepted for ASTAR-NIST, then this program has the best goodness of fit with experimental data. Among the computed statistic values, except ASTAR-NIST, the SRIM has a small value even its Chi distribution is higher than the other programs. The reason that SRIM has this distribution is due to more categories (number of points) that involved in the test. So even the null hypothesis is rejected, and we conclude that there is no goodness of fit between experimental and program data, but the second test declares that it is not as an inferior. Table (VIII) shows the result of the standard deviation test for the programs with experimental data. It enlightens that the SRIM has the lowest σ among other programs, including ASTAR-NIST that gave a better goodness of fit. As a summary, the two statistical tests give a similar result, despite the different bases on which it was established. The ASTAR-NIST has the best goodness of fit according to the first test and good agreement with experimental data are clustered nearly about the normalized mean difference and then the data are more reliable to match with experimental data compared to ASTAR-NIST.



Figure (2): Electronic stopping power verses Helium ions energy for (a) Aluminum Oxide (b) Carbon Dioxide for used programs and some of available experimental data (Santry & Werner 1986) and (Bourland *et al.* 1971), respectively.

Table (V): Chi-Square Test for Goodness-of-Fit at level 0.05 among experimental data (Santry & Werner 1986) and different programs for Helium ion bombarded Aluminum oxide.

Program	Hypothesis	Categories	Chi Squared	Distribution	P - value	Statistic
SRIM	False	23	33.924439035575	ChiSquared22	0	167.087
ASTAR - libdEdx	False	21	31.410433095525	ChiSquared20	0	6469.11
ASTAR - NIST	True	21	31.410433095525	ChiSquared20	0.305021	22.6752
ICRU49+73	False	21	31.410433095525	ChiSquared20	0	6469.11
BETHE_EXT00	False	21	31.410433095525	ChiSquared20	0	6121.59
MSTAR	False	21	31.410433095525	ChiSquared20	0	6469.56

 Table (VI): Standard deviation (STD) and mean normalized difference test among experimental data (Santry & Werner 1986) and different programs for Aluminum oxide bombarded by Helium ion.

Program	SRIM	ASTAR -dEdx	ASTAR - NIST	ICRU49+73	BETHE_EXT00	MSTAR
Energy MeV	0.2 -2	0.2 -2	0.2 -2	0.2 -2	0.2 -2	0.2 -2
No. of points	23	21	21	21	21	21
Δ	-7.2875	25.2539	-1.8043	25.2543	27.6922	25.1200
σ	± 3.5008	±27.1384	± 2.6370	±27.1387	±22.6855	± 27.3172

Table (VII): Chi-Square Test for Goodness-of-Fit at level 0.05 of experimental data (Bourland *et al.* 1971) with different programs for Helium ion bombarded Carbon Dioxide gas.

Program	Hypothesis	Categories	Chi Squared	Distribution	P - value	Statistic
SRIM	False	17	26.296227622047	ChiSquared16	0	121.233
ASTAR - dEdx	False	10	16.918977448709	ChiSquared9	0	6660.07
ASTAR - NIST	True	10	16.918977448709	ChiSquared9	0.759022	5.80747
ICRU49+73	False	10	16.918977448709	ChiSquared9	0	6658.07
BETHE_EXT00	False	10	16.918977448709	ChiSquared9	0	6195.2
MSTAR	False	10	16.918977448709	ChiSquared9	0	6661.03

Table (VIII): Standard deviation (STD) and mean normalized difference test of experimental data (Bourland *et al.* 1971) with different programs for Carbon Dioxide gas bombarded by Helium ion.

Program	SRIM	ASTAR -dEdx	ASTAR - NIST	ICRU49+73	BETHE_EXT00	MSTAR
Energy MeV	0.3 -2	0.3 -2	0.3 -2	0.2 -2	0.3 -2	0.3 -2
No. of points	17	10	10	10	10	10
Δ	6.0431	37.4113	-0.2957	37.4055	37.3385	37.4346
σ	± 1.2393	± 22.3483	± 1.9250	± 22.35360	± 20.3474	±22.3193

For the rest of this work, we choose Boron as an ion heavier than Helium to bombard two purely elements. Figure (3a) shows the ESP as a function of Boron ion energy for Aluminum using the programs and experimental data (Hsu et al. 2005), while Figure (3b) is for Gold with experimental data (Kuronen et al. 1988). Obviously, the ESP vs. energy for both elements shows that the SRIM has a wavy behavior at low energy region compared to the other programs. This can be attributed to the algorithm involved in calculations of heavier ions in the program. Figure (3a-b) shows the lack of ICRU49+37 curve extension in the lower energy for both elements. The program does not confine this low ion energy region. This might be systemically input imposes by both reports of ICRU. In spite of this defect in a curve, fortunately it does not affect our purpose of work because the handy experimental data for both elements are far from this range of energy. Table (IX) shows the results of the Chi square test for Boron ions bombarded Aluminum. Obviously, the test shows that there exists statistical evidence against the null hypotheses of all programs. The Chi distributions, categories and the χ^2 value are similar. There is a difference in the computed statistic values. The test shows a minuscule p-value for MSTAR that the test rejects the null hypothesis. We conclude that the experimental data are not well distributed with the programs. According to this test all programs fail to satisfy the goodness of fit. But this is a relative statement because ICRU49+73 and MSTAR have small computed statistic values compared to the two programs. Associating this argument with the second test, one can expect that ICRU49+73 and MSTAR would give a good agreement compared to the other two. This conclusion is confirmed by noticing Table (X) results in the standard deviation test. The ICRU49+73 and MSTAR have small values of σ . We argued that the goodness of fit would be closely analogical between ICRU49+73 and MSTAR. The second test elucidates that ICRU49+73 has more tradeoffs of good agreement over MSTAR due to smallest σ and then more accuracy with experimental data. The SRIM and BETHE-EXT00 due to their higher σ are far from agreement. On the other hand, for Gold bombarded by Boron ion, Table (XI) indicates that MSTAR has a higher degree of goodness of fit due to higher p-value. In spite of the rejection of null hypotheses, the ICRU49+37 has, in order, the less degree of goodness of fit compered to SRIM and BETHE-EXT00 due to lower computed statistic for fixed χ^2 value. Furthermore, Table (XII), points out that these programs have the best agreement with experimental data achieved by standard deviation test. However, this test gives the priority for a good agreement of the programs. The best agreement is for ICRU49+73, MSTAR, BETHE-EXT00, and SRIM, respectively.

Advances in Physics Theories and Applications ISSN 2224-719X (Paper) ISSN 2225-0638 (Online) Vol.66, 2017



Figure (3): Electronic stopping power verses Boron ions energy for (a) Aluminum (b) Gold for used programs and some of available experimental data (Hsu *et al.* 2005) and (Kuronen *et al.* 1988), respectively.

Table (IX): Chi-Square Test for Goodness-of-Fit at level 0.05 among experimental data (Hsu *et al.* 2005) and different programs for Boron bombarded Aluminum.

Program	Hypothesis	Categories	Critical value	Distribution	P - value	Statistic
SRIM	False	11	18.3070380532751	ChiSquare10	0	19855.3
ICRU49+73	False	11	18.3070380532751	ChiSquare10	0	104.406
BETHE_EXT00	False	11	18.3070380532751	ChiSquare10	0	2418.59
MSTAR	False	11	18.3070380532751	ChiSquare10	2.66104×10 ⁻	71.1472
				-	11	

Table (X): Standard deviation (STD) and mean normalized difference test among experimental data (Hsu *et al.*2005) and different programs for Boron bombarded Aluminum.

Program	SRIM	ICRU49+73	BETHE_EXT00	MSTAR
Energy MeV	0.1 – 0.6	0.1 – 0.6	0.1 – 0.6	0.1 – 0.6
No. of points	11	11	11	11
Δ	45.6127	-4.9744	13.4436	3.4384
σ	±12.3490	±1.0579	±15.0936	±2.2256

 Table (XI): Chi-Square Test for Goodness-of-Fit at level 0.05 among experimental data (Kuronen *et al.* 1988) and different programs for Boron bombarded Gold.

Program	Hypothesis	Categories	Critical value	Distribution	P - value	Statistic
SRIM	False	9	15.5073130558655	ChiSquare8	0	10852.6
ICRU49+73	False	9	15.5073130558655	ChiSquare8	1.2419×10 ⁻⁶	42.2004
BETHE_EXT00	False	9	15.5073130558655	ChiSquare8	0	5557.8
MSTAR	True	9	15.5073130558655	ChiSquare8	0.630832	6.14644

 Table (XII): Standard deviation (STD) and mean normalized difference test among experimental data (Kuronen et al. 1988) and different programs for Boron bombarded Gold.

Program	SRIM	ICRU49+73	BETHE_EXT00	MSTAR
Energy MeV	0.316 - 0.639	0.316 - 0.639	0.316 - 0.639	0.316 - 0.639
No. of points	9	9	9	9
Δ	59.3056	5.3012	48.1835	3.4384
σ	±5.1668	±2.1081	<u>+</u> 4.5062	±2.2256

4. Conclusion

Sometimes graphs are not sufficient to describe whether the experimental and theoretical data are consistent. Therefore, statistical tests are used to show the degree of conformity between them, especially when the points of these programs are very close to the corresponding experimental data. The reason that various programs assign different ESPs for the same ion-material combinations is due to different manner, mathematical formulas and the

parameters involved. Two statistical tests used to confirm that a certain program gives well approval between experimental and program data for specific ion- material combinations, may come to fail in the other combinations. The two statistical tests proved that they are identical in their strength to find out the harmony between experimental and programs data.

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