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ELECTRONIC STOPPING POWER OF VARIOUS ORGANIC COMPOUNDS FOR PROTON (0.05-10 MeV): A COMPARATIVE STUDY

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Abstract. Electronic stopping power of various organic compounds for proton (0.05-10 MeV) calculated using different theoretical and semi-empirical formulations has been analysed in the present investigation. The stopping power values calculated using Ashley's dielectric model (ADM) with evaluation approach for optical energy loss function (OELF) have been compared with the values computed using the theoretical formulation CasP (Convolution approximation for swift Particles) and semi-empirical approach SRIM (Stopping and Range of Ions in Matter). The merits and demerits of the adopted formulations are highlighted in the present energy region. These type of stopping power analyses for proton will be helpful for scientific community to choose best formulation.

1. Introduction

The effective and successful applications of the radiation technology require a detailed knowledge about the different processes involved during the interaction of the charged particle with matter. Various analyses, developments and modifications have continuously influenced the theoretical, semi-empirical and experimental ideas for the deep understanding of radiation interaction [1-19]. Stopping of light ions like protons in matter has been a subject of great theoretical and experimental interest. The proton energy loss calculation for different complex media constitutes information essential for important applications in radiation physics, chemistry, biology, medicines and therapies. Protons beam represent an exploring radiotherapy alternative for efficient treatment of tumours [20-24]. The accurate dosimetry of proton radiation depends on a detailed knowledge of proton stopping power in the material of interest. In many situations, the accuracy of the material response determination is limited by the accuracy of various range and stopping power calculations. The experimental range and energy loss data for various ion/material combinations have been produced but for most of the complex organic compounds, rare number of stopping data for protons are available.

In the present investigation, the stopping power of some important organic materials (polypropylene, Polycarbonate, Mylar, Polyvinylalcohol, Poly-oxymethlylene, Polyacrylonitrile, Polyvinylpyrrolidone, Polyvinylacetate, Kapton and Bakelite) for proton (10-10000 KeV) calculated using the Ashley's dielectric model (ADM) with evaluation approach for optical energy loss function (OELF) [25-29] have been compared with the values calculated using the theoretical formulation CasP (Convolution approximation for swift Particles) [19] and semi-empirical approach SRIM (Stopping and Range of Ions in Matter) [17]. The merits and demerits of the adopted formulations are highlighted in the adopted energy region.

2. Stopping Power Formulations

In the present work, three different formulations (ADM; CasP4.0; SRIM08.04) [15, 17, 25-29] have been used to analyse the stopping power calculations of different complex organic compounds [polypropylene (C_3H_6; ρ=0.9 gm/cm^3), Polycarbonate ($C_{16}H_{14}O_3$; ρ=1.2 gm/cm^3), Mylar ($C_{10}H_8O_4$; ρ=1.4 gm/cm^3), Polyvinylalcohol ($C_2H_4O_1$; ρ=1.3 gm/cm^3), Poly-oxymethlylene ($C_1H_2O_1$; ρ= 1.425 gm/cm^3), Polyacrylonitrile ($C_3H_3O_1$; ρ=1.17 gm/cm^3), Polyvinylpyrrolidone ($C_6H_9N_1O_1$; ρ=1.25 gm/cm^3), Polyvinylacetate ($C_4H_6O_2$; ρ=1.19 gm/cm^3), Kapton ($C_{22}H_{10}N_2O_5$; ρ=1.42 gm/cm^3), Bakelite ($C_{44}H_{36}O_6$; ρ=1.4 gm/cm^3)] for proton in the energy region of 50-10000 KeV [29]. The values calculated using Ashley's dielectric model (ADM) [30], with evaluation approach of optical energy loss functon (OELF) [25-29] have been compared with the famous theoretical approach (CasP) by Grande and Schiweitz [19] and semiempirical formulation (SRIM) by Ziegler [17].

The stopping power values calculated By Tan et al., [29] using the Ashley's dielectric model (ADM) with evaluation approach for optical energy loss function (OELF) have been expressed in three terms [25-29] as given by

$$SP = SP_b + SP_{BEC} + SP_{BC},$$

where SP_b is the basic stopping power according to Ashley [30], SP_{BEC} is the barkas-effect correction, and SP_{BC} is the Bloch correction in the stopping power calculation [29]. The optical energy loss function (OELF) is evaluated using the empirical (analysis of the structure features) method [25-29]. There is need to check the reliability of this approach by comparing the values calculated using the other well developed and available approaches (SRIM and CasP) [17, 19]. For this purpose, we have used the stopping power values of ten organic compounds for proton calculated by Tan et al. [29].

CasP (Convolution approximation for swift Particles) program avoids the effective-charge postulate and hence does not make use of input based on stopping experiments. This program [19] makes use of the convolution approximation (either the perturbative convolution approximation PCA or the more advanced unitary convolution approximation UCA). The unitary convolution approximation (UCA), a non-linear theory includes an approximation to the wave packet formalism by Bloch [31-33], and thus each electron is counted only once in a collision and ionization probabilities are restricted to a maximum of 100 %. The code is based on an exact matching of the quantum mechanical mean electronic energy transfers for the asymptotic region of very low and very high energy transfers to the target electron similar as in the Bethe or in the Bloch theory. The total electronic energy loss cross section (equivalent to stopping power) is subsequently calculated from the mean electronic energy transfer, which is a function of impact parameter. The computation of these two (mean electronic energy transfer and total electronic energy-loss cross section) accounts for a selected predefined projectile-screening function.

In version CasP3.1, polarization effects (e.g. the barkas effect) are not included but some new modifications (extended Bragg's additivity rule for compounds, new solid/gas target selection, improved accuracy for the kernel integration in the case of *K* shells of very heavy atoms such as uranium) have been implemented.

In version 3.2 (CasP3.2) new modifications [Improved relativistic correction accounted for the impact-parameter dependence, new projectile-electron loss (energy losses due to projectile ionization and excitation) option now also for compounds, new MEIS (Medium Energy Ion-Scattering) energy-loss parameter output] have been implemented. In CasP4.0 [19, 32-37], Modification on Bloch and Shell corrections are implemented, internal charge number for the UCA scaling for screened projectiles is improved, close collision function is

replaced by an accurate fit formula, improved the accuracy for deeply bound inner shell by introducing new gridding, improved a model for the energy-loss spreading at b=0, the Barkas effect for close non-Coulombic collisions has been included, possible direct selection of the projectile charge-state is implemented and the speed of stopping cross-section calculations has also been improved.

SRIM (Stopping and Range of Ions in Matter) is a group of programs [17], which calculates the range and stopping of ions (up to 2 GeV/n) into matter using a quantum mechanical treatment of ion-atom collisions [1]. Electronic stopping powers are deduced from those for protons by means of an effective-charge fraction assumed to be independent of the target. The charge state of the ion within the target is described using the concept of effective charge [38], which includes a velocity dependent state and long-range screening due to the collective electron sea of the target [1]. Low velocity stopping powers are not necessarily assumed to be velocity proportional but different power-laws, dependent on Z_1 and Z_2 have been adopted. Stopping powers for compounds are determined on the basis of an extensive study of experimental data for proton, helium and lithium projectiles [39].

Major changes occur in SRIM about every 5 years. In SRIM2008 [40] many small bugs have been corrected, it is now possible to add range and damage spectra from different ions at different energies and angles into a single spectra, during the TRIM calculation, one can Pause TRIM, and then Change TRIM, has the option of adding the new data to the old data-files has been implemented.

It seems therefore appropriate to present a comparative analysis of these three approaches for the stopping power calculation of ten different organic materials for protons in the energy region of 50-10000 KeV.

3. Results and Discussion

The electronic stopping power of a group of ten different organic compounds for proton in the enegy region (0.05-10 MeV) calculated using these three adopted formulations (ADM; CasP4.0; SRIM08.04) [17, 19, 29] are presented in the Tables 1-10. Figures (1-10) show the comparison of these calculated stopping power values in the energy region (50-500 KeV) for clear visualisation of the deviations.

Table 1 presents the stopping power of polypropylene (C_3H_6; ρ=0.9 gm/cm^3) calculated using the different adopted approaches (ADM; CasP4.0; SRIM08.04) for proton (0.05-10 MeV). For polypropylene, it is clear from the given table that at higher energy region, all the adopted formulations show overall same results of stopping power values. At lower energy region (50-100 KeV), all these formulations deviated significantly from each other (Fig. 1). The values predicted by SRIM [17] and Ashley's approach show the overall same results except for 50 and 60 KeV protons. The CasP tabulated stopping power values at this low energy region deviate from the values predicted by the other two approaches.

Table 2 shows the stopping power of Polycarbonate ($C_{16}H_{14}O_3$; ρ=1.2 gm/cm^3) for proton (0.05-10 MeV). As we have observed for polypropylene, same trend is observed for polycarbonate. At higher energy region, there is very few deviation between the values predicted by all the three adopted procedures. At lower energy region (50-100 KeV) of proton, the values deviate significantly from each other. The convolution approach of Grande and Schiwietz [19] predicts much less stopping power values as compared to SRIM and Ashley's approaches in this low energy region. The deviation shown by the values predicted by CasP4.0 and ADM from the semi-empirical SRIM formulation increases as the energy of the proton decreases. For rest of the organic materials (Tables 3-10 and Figs. 3-10), same trend is observed by all the adopted formulations.

Table 1. Stopping power (eV/Å) of polypropylene for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	8.033	9.822	5.302
60	9.556	9.980	5.975
70	10.18	9.998	6.562
80	10.34	9.914	7.072
90	10.25	9.758	7.496
100	10.03	9.555	7.830
150	8.631	8.311	8.202
200	7.476	7.191	7.451
300	5.870	5.648	5.935
400	4.853	4.698	4.952
500	4.155	4.059	4.274
600	3.669	3.597	3.776
700	3.318	3.248	3.394
800	3.038	2.973	3.091
900	2.807	2.751	2.844
1000	2.614	2.569	2.638
1500	1.963	1.997	1.967
2000	1.588	1.615	1.588
3000	1.165	1.180	1.168
4000	0.9290	0.9403	0.9334
5000	0.7773	0.7870	0.7828
6000	0.6709	0.6797	0.6769
7000	0.5917	0.6001	0.5980
8000	0.5303	0.5384	0.5369
9000	0.4813	0.4892	0.4880
10000	0.4411	0.4489	0.4481

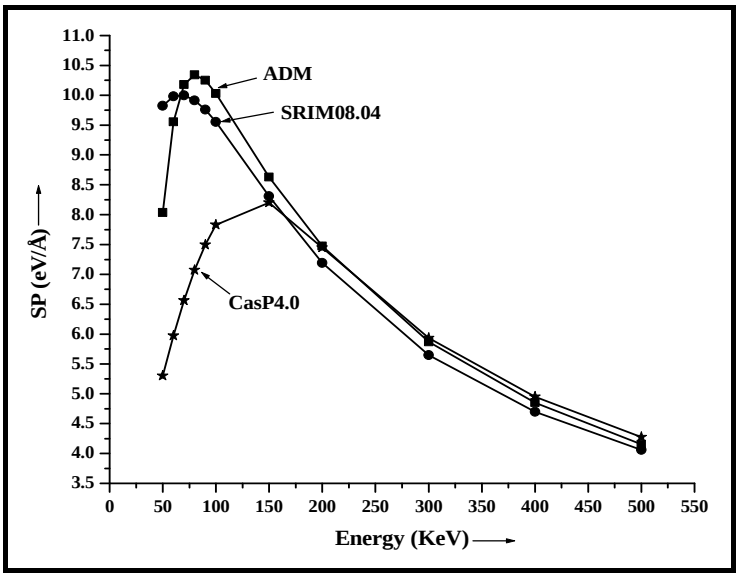

Fig. 1. Stopping power (eV/Å) of polypropylene for proton in the energy range of 0.05-0.5 MeV.

Table 2. Stopping power (eV/Å) of polycarbonate for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	7.038	9.731	5.666
60	9.098	9.981	6.387
70	10.08	10.09	7.020
80	10.45	10.09	7.574
90	10.52	10.00	8.040
100	10.42	9.861	8.418
150	9.29	8.795	8.946
200	8.188	7.729	8.236
300	6.542	6.185	6.640
400	5.457	5.200	5.578
500	4.696	4.526	4.837
600	4.161	4.034	4.286
700	3.774	3.658	3.862
800	3.463	3.361	3.524
900	3.206	3.121	3.249
1000	2.989	2.922	3.019
1500	2.265	2.28	2.261
2000	1.843	1.859	1.837
3000	1.361	1.371	1.358
4000	1.09	1.098	1.090
5000	0.9144	0.922	0.9159
6000	0.7906	0.7982	0.7938
7000	0.6983	0.7059	0.7023
8000	0.6266	0.6343	0.6313
9000	0.5692	0.5770	0.5750
10000	0.5221	0.5300	0.5280

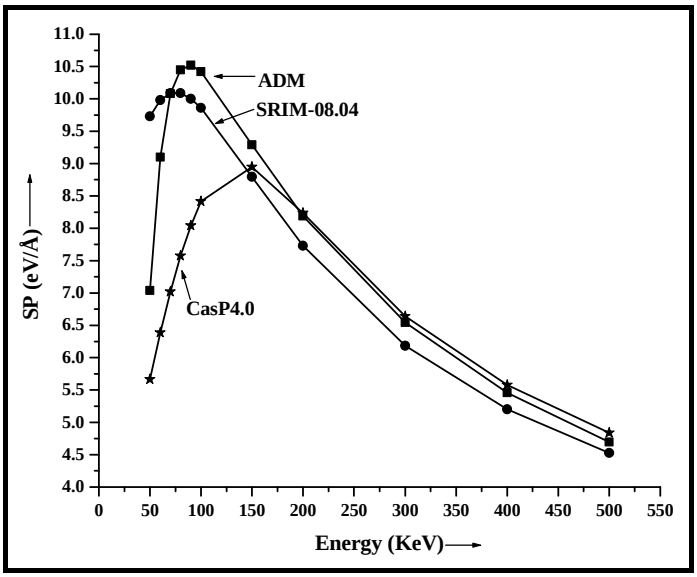

Fig. 2. Stopping power (eV/Å) of polycarbonate for proton in the energy range of 0.05-0.5 MeV.

Table 3. Stopping power (eV/ Å) of Mylar for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	7.056	10.26	6.220
60	9.457	10.56	7.024
70	10.63	10.71	7.731
80	11.12	10.74	8.350
90	11.27	10.61	8.881
100	11.23	10.56	9.311
150	10.20	9.491	9.983
200	9.067	8.378	9.254
300	7.31	6.733	7.498
400	6.128	5.675	6.317
500	5.290	4.948	5.479
600	4.693	4.418	4.860
700	4.254	4.013	4.383
800	3.902	3.694	4.001
900	3.610	3.438	3.690
1000	3.363	3.228	3.429
1500	2.554	2.560	2.565
2000	2.082	2.102	2.088
3000	1.541	1.555	1.545
4000	1.236	1.247	1.241
5000	1.038	1.048	1.044
6000	0.8979	0.9078	0.9048
7000	0.7935	0.8032	0.8008
8000	0.7123	0.7220	0.7204
9000	0.6472	0.6570	0.6554
10000	0.5938	0.6035	0.6027

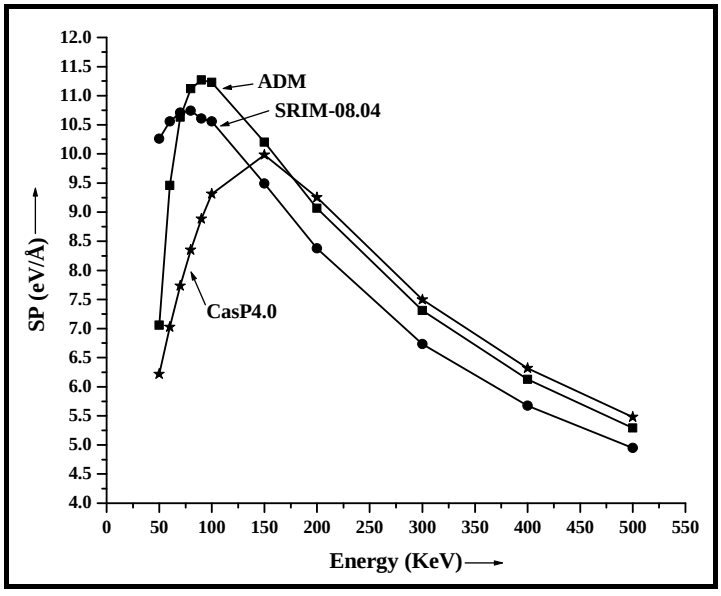

Fig. 3. Stopping power (eV/ Å) of Mylar for proton in the energy range of 0.05-0.5 MeV.

Table 4. Stopping power (eV/ Å) of Polyvinylalcohol for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	8.442	11.66	6.460
60	10.62	11.95	7.297
70	11.60	12.06	8.036
80	11.94	12.04	8.682
90	11.98	11.92	9.233
100	11.86	11.73	9.680
150	10.59	10.39	10.34
200	9.338	9.089	9.540
300	7.479	7.217	7.696
400	6.252	6.039	6.460
500	5.389	5.238	5.591
600	4.770	4.656	4.953
700	4.312	4.213	4.456
800	3.945	3.863	4.061
900	3.642	3.580	3.740
1000	3.387	3.346	3.471
1500	2.558	2.614	2.585
2000	2.079	2.122	2.094
3000	1.534	1.559	1.547
4000	1.228	1.246	1.240
5000	1.030	1.045	1.0411
6000	0.8902	0.9042	0.9018
7000	0.7862	0.7993	0.7975
8000	0.7054	0.7179	0.7168
9000	0.6406	0.6528	0.652
10000	0.5875	0.5994	0.5992

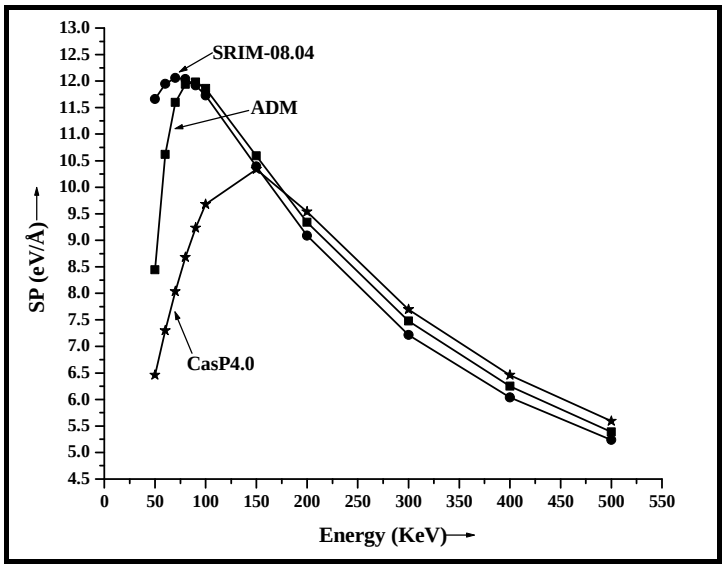

Fig. 4. Stopping power (eV/ Å) of polyvinylalcohol for proton in the energy range of 0.05-0.5 MeV.

Table 5. Stopping power (eV/ $\mathring{A}$) of Poly-oxymethlylene for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	7.618	11.38	6.472
60	10.01	11.73	7.319
70	11.13	11.89	8.074
80	11.57	11.91	8.737
90	11.70	11.84	9.312
100	11.67	11.69	9.781
150	10.66	10.47	10.56
200	9.499	9.215	9.827
300	7.695	7.364	7.985
400	6.472	6.183	6.724
500	5.600	5.376	5.831
600	4.964	4.788	5.171
700	4.486	4.338	4.656
800	4.102	3.983	4.247
900	3.785	3.696	3.906
1000	3.519	3.459	3.629
1500	2.664	2.722	2.702
2000	2.171	2.218	2.199
3000	1.608	1.634	1.624
4000	1.289	1.309	1.303
5000	1.082	1.099	1.095
6000	0.9366	0.9515	0.9495
7000	0.8277	0.8416	0.8406
8000	0.7430	0.7564	0.7556
9000	0.6751	0.6881	0.6878
10000	0.6194	0.632	0.6323

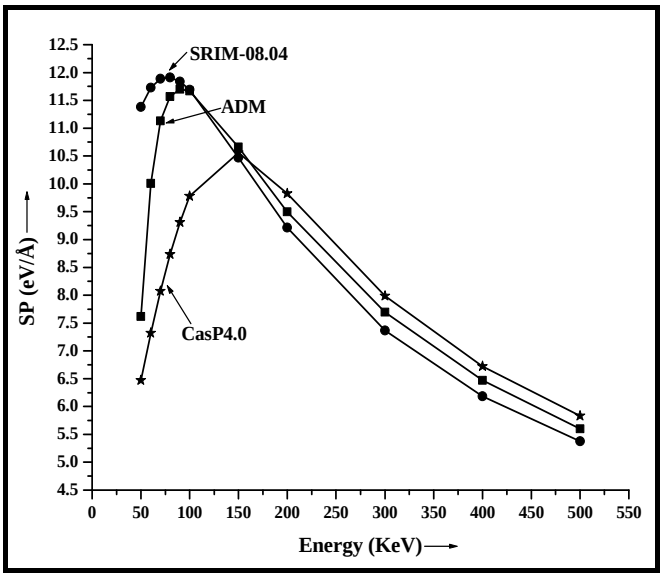

Fig. 5. Stopping power (eV/ $\mathring{A}$) of poly-oxymethylene for proton in the energy range of 0.05-0.5 MeV.

Table 6. Stopping power (eV/ Å) of Polyacrylonitrile for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	7.202	10.03	5.672
60	9.21	10.27	6.397
70	10.16	10.36	7.029
80	10.51	10.34	7.4074
90	10.56	10.24	8.040
100	10.44	10.08	8.410
150	9.250	8.929	8.896
200	8.122	7.811	8.171
300	6.474	6.218	6.567
400	5.390	5.213	5.511
500	4.633	4.528	4.773
600	4.099	4.029	4.228
700	3.710	3.647	3.809
800	3.400	3.345	3.475
900	3.149	3.099	3.204
1000	2.939	2.895	2.976
1500	2.228	2.249	2.232
2000	1.811	1.828	1.810
3000	1.337	1.346	1.337
4000	1.070	1.077	1.073
5000	0.8971	0.9044	0.9021
6000	0.7755	0.7828	0.7814
7000	0.6848	0.6922	0.6913
8000	0.6144	0.6219	0.6214
9000	0.558	0.5656	0.5652
10000	0.5117	0.5195	0.5147

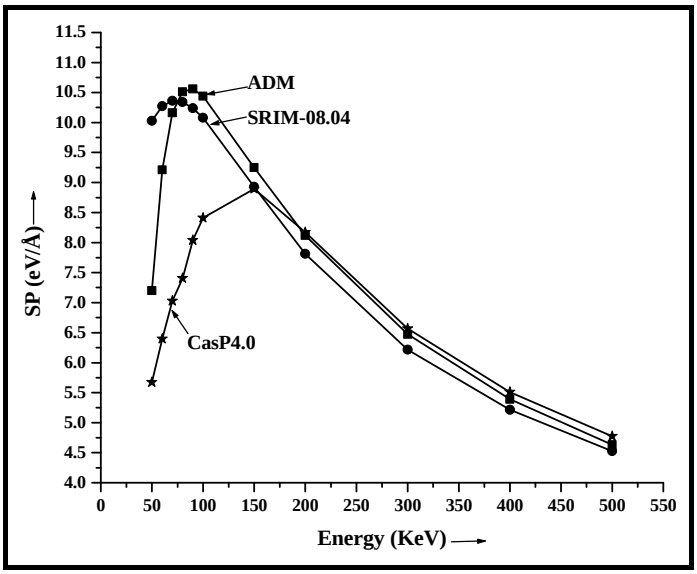

Fig. 6. Stopping power (eV/ Å) of Polyacrylonitrile for proton in the energy range of 0.05-0.5 MeV.

Table 7. Stopping power (eV/Å) of Polyvinylpyrrolidone for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	8.317	10.67	6.283
60	10.43	10.92	7.085
70	11.39	11.01	7.797
80	11.72	10.97	8.407
90	11.74	10.86	8.929
100	11.60	10.68	9.350
150	10.26	9.433	9.912
200	9.010	8.237	9.105
300	7.181	6.539	7.316
400	5.982	5.474	6.141
500	5.145	4.751	5.314
600	4.552	4.229	4.704
700	4.117	3.832	4.235
800	3.770	3.523	3.861
900	3.486	3.276	3.556
1000	3.248	3.075	3.302
1500	2.455	2.46	2.467
2000	1.994	2.018	2.000
3000	1.470	1.487	1.476
4000	1.176	1.189	1.183
5000	0.9863	0.9976	0.9930
6000	0.8524	0.8631	0.8600
7000	0.7526	0.7629	0.7610
8000	0.6751	0.6852	0.6830
9000	0.6131	0.6231	0.6220
10000	0.5622	0.5721	0.5720

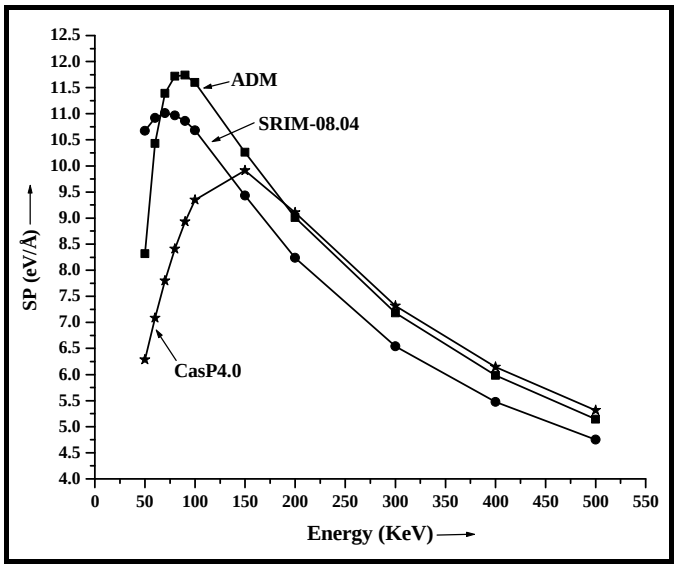

Fig. 7. Stopping power (eV/Å) of Polyvinylpyrrolidone for proton in the energy range of 0.05-0.5 MeV.

Table 8. Stopping power (eV/ Å) of Polyvinylacetate for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	7.008	9.958	5.621
60	9.022	10.23	6.343
70	9.958	10.34	6.991
80	10.31	10.35	7.554
90	10.38	10.26	8.035
100	10.30	10.12	8.422
150	9.256	9.022	9.021
200	8.186	7.920	8.338
300	6.575	6.320	6.7498
400	5.504	5.303	5.675
500	4.748	4.609	4.918
600	4.206	4.103	4.359
700	3.806	3.716	3.925
800	3.484	3.41	3.579
900	3.219	3.162	3.298
1000	2.995	2.957	3.063
1500	2.267	2.307	2.284
2000	1.844	1.876	1.857
3000	1.363	1.381	1.370
4000	1.092	1.105	1.099
5000	0.9163	0.8604	0.9238
6000	0.7924	0.803	0.8006
7000	0.7000	0.7101	0.7083
8000	0.6282	0.6381	0.6368
9000	0.5706	0.5803	0.5794
10000	0.5234	0.533	0.5326

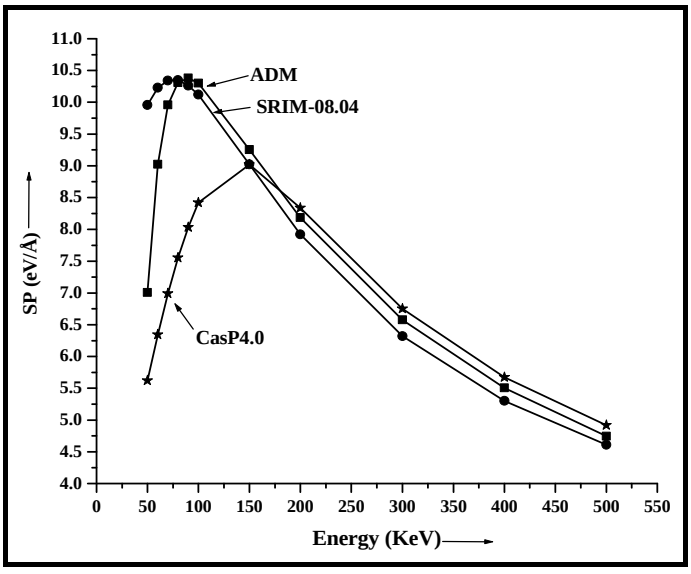

Fig. 8. Stopping power (eV/ Å) of Polyvinylacetate for proton in the energy range of 0.05-0.5 MeV.

Table 9. Stopping power (eV/ Å) of Kapton for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	6.717	10.30	6.200
60	9.186	10.61	6.993
70	10.44	10.77	7.690
80	10.97	10.8	8.301
90	11.15	10.75	8.819
100	11.12	10.62	9.240
150	10.11	9.567	9.869
200	8.978	8.456	9.139
300	7.232	6.812	7.399
400	6.055	5.750	6.234
500	5.223	5.018	5.412
600	4.634	4.481	4.803
700	4.205	4.070	4.333
800	3.861	3.744	3.958
900	3.577	3.479	3.651
1000	3.338	3.261	3.394
1500	2.540	2.551	2.545
2000	2.072	2.087	2.0731
3000	1.534	1.545	1.536
4000	1.230	1.239	1.234
5000	1.033	1.042	1.038
6000	0.8941	0.9029	0.9000
7000	0.7901	0.7991	0.7970
8000	0.7093	0.7184	0.7170
9000	0.6446	0.6538	0.6530
10000	0.5914	0.6007	0.6000

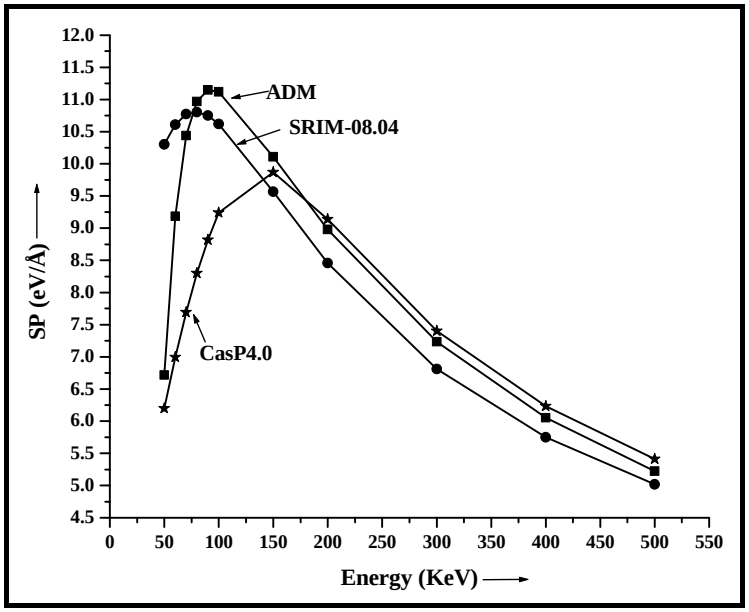

Fig. 9. Stopping power (eV/ Å) of Kapton for proton in the energy range of 0.05-0.5 MeV.

Table 10. Stopping power (eV/Å) of Bakelite for proton in the energy range of 0.05-10 MeV.

Energy (KeV)	ADM [29]	SRIM-08.04 [17]	CasP4.0 [19]
50	8.248	12.09	6.666
60	10.65	12.37	7.514
70	11.78	12.48	8.256
80	12.22	12.45	8.900
90	12.29	12.33	9.445
100	12.17	12.14	9.880
150	10.85	10.77	10.48
200	9.556	9.433	9.639
300	7.626	7.523	7.760
400	6.356	6.314	6.519
500	5.467	5.488	5.649
600	4.844	4.887	5.008
700	4.396	4.427	4.513
800	4.036	4.063	4.120
900	3.738	3.769	3.798
1000	3.486	3.525	3.530
1500	2.642	2.735	2.643
2000	2.149	2.223	2.148
3000	1.587	1.636	1.587
4000	1.271	1.309	1.274
5000	1.066	1.099	1.071
6000	0.9216	0.9507	0.9279
7000	0.8140	0.8406	0.8209
8000	0.7304	0.7551	0.7381
9000	0.6634	0.6867	0.6714
10000	0.6085	0.6306	0.6172

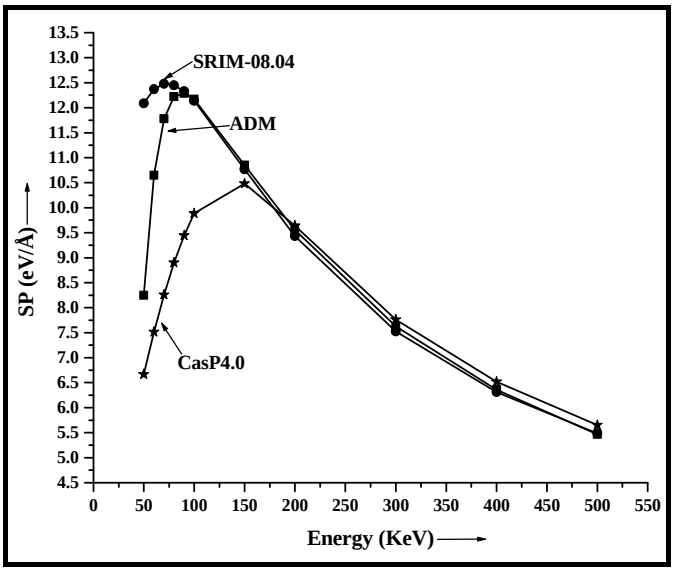

Fig. 10. Stopping power (eV/Å) of Bakelite for proton in the energy range of 0.05-0.5 MeV

From these comparative analyses, it is interesting to note that the semi-empirical formulation SRIM and Ashley's dielectric model (ADM) provide maximum accurate stopping power values for important organic materials for proton in the energy region (0.05-10 MeV). It is well known that the SRIM formulation has established very reliable and reputed procedure for range and stopping power for all types of material/ion combinations. Ashley's dielectric model with the evaluation approach for optical energy loss function (OELF) provide better stopping power results as compared to theoretical approach CasP.

4. Conclusion

From this comparative analysis, it can be concluded that the stopping power values predicted by various formulations for important organic material/proton combination provide valuable information which can play an important role in material analyses and different successful applications. The formulations like SRIM and Ashley's dielectric model (ADM) provide reliable and accurate results of stopping power for various organic material/proton combinations as compared to CasP code. These type of analyses are very helpful for scientific community. For most of the organic compounds/proton combinations, various stopping power formulations for energy below 70 KeV should be analyse to highlight the best procedure of stopping power.

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