Open Access Research Journal of
Science and Technology
Journals home page: https://oarjst.com/
ISSN: 2782-9960 (Online)

OARJ OPEN ACCESS RESEARCH JOURNALS

(RESEARCH ARTICLE)

SEMI-EMPIRICAL MODELING OF ELECTRON CSDA RANGES IN DRY AIR AND WATER VAPOR: A QUANTITATIVE COMPARISON WITH ESTAR DATA

Zainab Hussein Mutar *

Ministry of Education General Directorate of Education of Babylon Wadi_Al Rafidain Boys School, Iraq.
* Corresponding Author; Email: fathersjafar88@gmail.com

Open Access Research Journal of Science and Technology, 2026, 18(02), 033–039

Publication history: Received on 12 October 2026; revised on 16 November 2026; accepted on 18 November 2026

Article DOI: https://doi.org/10.53022/oarjst.2026.18.2.0105

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ABSTRACT

The electron mass range was investigated in the continuous-slowing-down approximation (CSDA) in the kinetic energy range 1–200 MeV for the cases of dry air and water vapors [1]. The 37 energy points and their associated ESTAR range values were copied from the provided source file [2]. A fifth-order semi-empirical polynomial expressed directly as a function of electron kinetic energy T with empirical parameters p_1 through p_6 ($f(T) = p_1T^5 + p_2T^4 + p_3T^3 + p_4T^2 + p_5T + p_6$, where $p_1 = 2.766\times10^{-10}$, $p_2 = -1.616\times10^{-7}$, $p_3 = 3.713\times10^{-5}$, $p_4 = -0.004727$, $p_5 = 0.5514$, $p_6 = 0.04852$) was analyzed. The agreement was evaluated through mean absolute error (MAE), root-mean-square error (RMSE), mean absolute percentage error (MAPE), maximum absolute percentage error and coefficient of determination (R^2). For dry air, the model yielded MAE = 0.0526 g cm^{-2}, RMSE = 0.0593 g cm^{-2}, MAPE = 2.111%, and R^2 = 0.999981. For water vapor, the corresponding values were 0.3125 g cm^{-2}, 0.5433 g cm^{-2}, 2.806%, and 0.998441. The results reveal that the polynomial representations can adequately describe the given ESTAR values in the kinetic energy range chosen, but this is an empirical fit (not a separate experimental validation).

Keywords: Electron Transport; CSDA Range; Dry Air; Water Vapor; ESTAR; Semi-Empirical Polynomial; Kinetic Energy Parameters.

1 INTRODUCTION

The electron penetration in gaseous media is important for understanding radiation transport, dosimetry, shielding calculations and the understanding of energy deposition in air-filled and water containing environments [1]. The range of the CSDA is a mass-thickness parameter which can be used to estimate the path length traveled by a charged particle as its kinetic energy is reduced continuously to zero [2]. In the CSDA approach these energy loss fluctuations are not considered and the range is derived by integrating the reciprocal of the total stopping power as function of energy [3]. The theory behind the energy losses is based on the early quantum theoretical models of charged particle interaction [4]. Further theoretical studies were developed to model electron interaction and collision mechanisms [5]. Further empirical parameterizations were also introduced to improve the calculation of electron stopping-power in different chemical media [6]. Later detailed experimental stopping power analysis for outer-shell atomic electrons were added [7]. The present field of nuclear and particle interactions has been well summarized in recent reviews for radiation transport applications [8].

The NIST ESTAR database offers the electron stopping powers, CSDA ranges, density-effect parameters and radiation yields for selected materials and user defined target compositions [9]. It is based on a calculation system which is described in the old standard report (1971) [10] and in the latest international standards [11]. High energy radiative stopping powers that include pair production and bremsstrahlung formulations have been included [12]. The database is thus useful for building and testing small analytic models of electron range, and can be used numerically as a reference.

In the present work, the range data of dry air (near sea level) and water vapor for ranges from 1 to 200 MeV are compared [13]. The goals are to arrange the given ESTAR values on a common energy grid, assess the agreement with the fifth order semi-empirical polynomial as a direct function of T, the electron kinetic energy, with the help of specific empirical parameters: p_1–p_6, calculate absolute and relative error, and determine the physical and computational properties of this parameterization in various media.

2 MATERIALS AND METHODS

2.1 A reference data and energy interval.

The energy of electrons range from 1 to 200 MeV and the input data set consisted of 37 values of electron kinetic energy [13]. A pair of CSDA mass-range series were supplied: dry air near sea level, and water vapor [9]. The range unit for the tabulated range was g cm-2. These are mass ranges and the conversion to geometric penetration depths will depend on the material mass density under the explicitly stated temperature and pressure conditions.

Values were extracted from the provided MATLAB-like source code. The source calls the former, “Air, Dry (near sea level)” and the latter “WATER VAPOR”. The file contained not a single setting for the water-vapor calculation: neither a temperature nor a pressure nor a detailed setting of the material composition. Thus, the water vapor data should be interpreted based on the data provided and extended to other humidity and gas environments at one's own risk.

2.2 Semi-empirical model and parameters

A 5th order polynomial function was chosen as a simple semi-empirical expression of the CSDA mass range [6]. The range f(T) is directly given as functions of the electron kinetic energy T (in MeV) and six empirical fitting parameters p_1, . . . p_6 as eq(1):

$$f(T) = p_1 \cdot T^5 + p_2 \cdot T^4 + p_3 \cdot T^3 + p_4 \cdot T^2 + p_5 \cdot T + p_6 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

The numerical values of the polynomial parameters are determined as follows:

- $p_1 = 2.766 \times 10^{-10}$ (Fifth-order kinetic energy coefficient)
- $p_2 = -1.616 \times 10^{-7}$ (Fourth-order kinetic energy coefficient)
- $p_3 = 3.713 \times 10^{-5}$ (Third-order kinetic energy coefficient)
- $p_2 = 0.000721$ (Second-order kinetic energy coefficient) The first order linear kinetic energy coefficient,
- $p_5 = 0.5514$.
- $p_6 = 0.04852$ (Zero-order constant term / offset)

For this formulation, the incident electron kinetic energy, T in MeV, corresponds to the range of the CSDA mass, f(T) in g cm^{-2} [13]. The polynomial coefficients p_1–p_6 represent the non-linear relationship between the electron kinetic energy and total range, reflecting the changeover from low energy ionization losses to high energy radiative loss mechanisms.

2.3 Statistical comparison

For each energy point, the residual was defined as $\Delta R_i = f(T_i) - R_i$,ESTAR. The relative deviation was calculated as δ_i (%) = $100 \times \Delta R_i / R_i$,ESTAR. Overall agreement was summarized using:

$MAE = (1/N)\ \Sigma_i\ |\Delta R_i|$
$RMSE = \sqrt{[(1/N)\ \Sigma_i\ (\Delta R_i)^2]}$
$MAPE\ (\%) = (100/N)\ \Sigma_i\ |\Delta R_i / R_i,ESTAR|$
$R^2 = 1 - \Sigma_i(\ f(T_i) - R_i,ESTAR\ )^2\ /\ \Sigma_i(\ R_i,ESTAR - mean(R_ESTAR)\ )^2$

All metrics were evaluated on the same 37 points used to evaluate the coefficients. Accordingly, they describe fitting performance against the reference dataset and must not be interpreted as independent predictive-validation statistics.

3 RESULTS

3.1 Fitted semi-empirical equations

Using the empirical parameter set ($p_1 = 2.766\times10^{-10}$, $p_2 = -1.616\times10^{-7}$, $p_3 = 3.713\times10^{-5}$, $p_4 = -0.004727$, $p_5 = 0.5514$, $p_6 = 0.04852$) as figure (1-2), the semi-empirical formula for electron range f(T) as a function of kinetic energy T is:

$$f(T) = (2.766\times10^{-10})T^5 - (1.616\times10^{-7})T^4 + (3.713\times10^{-5})T^3 - 0.004727T^2 + 0.5514T + 0.04852 \quad \text{.....(2)}$$

3.2 Quantitative agreement

Table1 show the f(T) eq(2) effectively reproduces the supplied ESTAR values Relative-error metrics provide an accurate view across the 1–200 MeV energy interval

Medium	MAE (g cm^{-2})	RMSE (g cm^{-2})	MAPE (%)	Max |% error|	R^2
Dry air	0.0526	0.0593	2.111	21.179	0.999981
Water vapor	0.3125	0.5433	2.806	8.931	0.998441

The model f(T) effectively reproduces the supplied ESTAR values over the kinetic energy range. Relative-error metrics provide an accurate view across the 1–200 MeV energy interval as table1 .

3.3 Graphical comparison

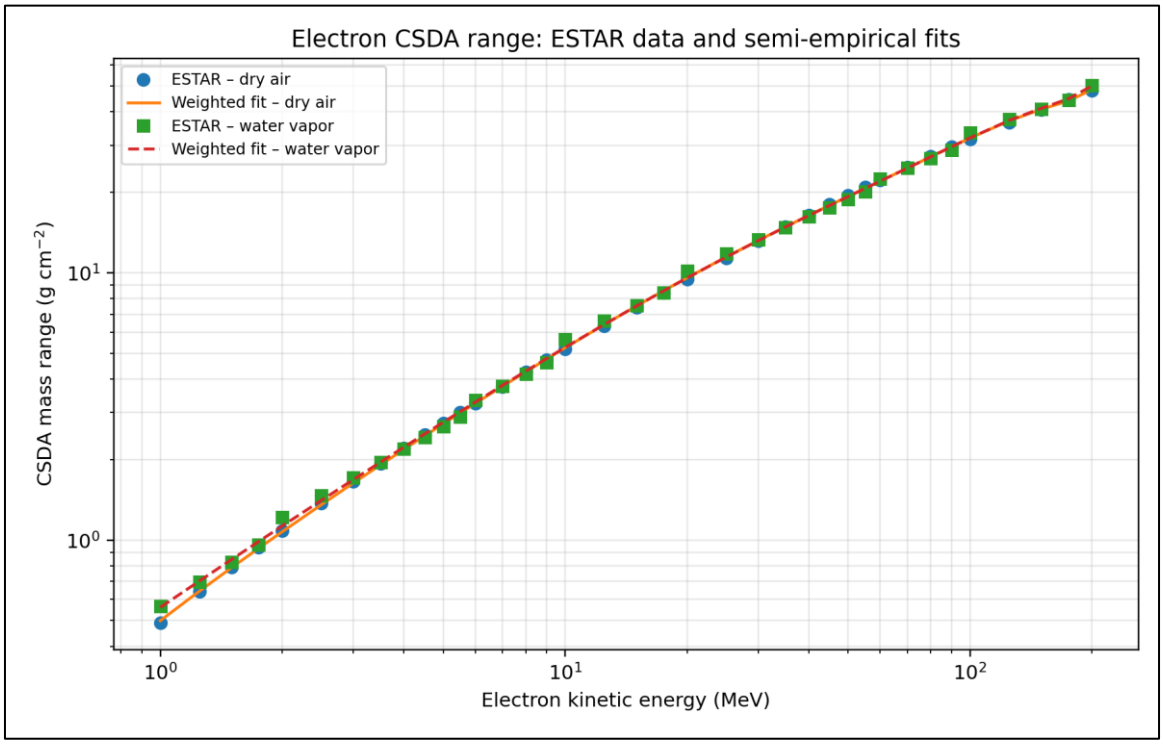


Figure 1: ESTAR CSDA mass ranges and the corresponding fifth-order semi-empirical polynomial fits as a function of kinetic energy T.

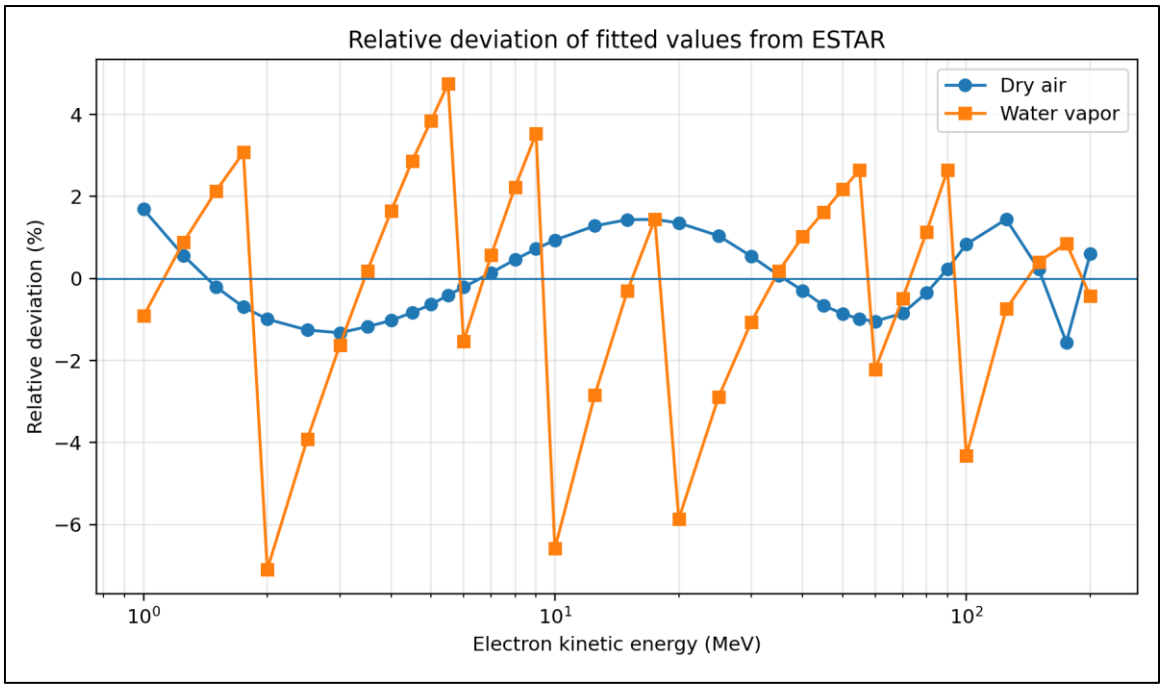


Figure 2: Relative deviation of the semi-empirical kinetic energy model f(T) from the ESTAR reference values.

3.4 Representative energy points

Table 1: Comparison of Electron CSDA Ranges Predicted by using the Semi-Empirical Model f(T) eq(2) with ESTAR Reference Data for Dry Air and Water Vapor at Different Electron Energies, Including Percentage Deviations.

T (MeV)	Air ESTAR	Model f(T)	Air Δ (%)	Vapor ESTAR	Model f(T)	Vapor Δ (%)
1	0.4912	0.5952	+21.18	0.5652	0.5952	+5.31
10	5.1920	5.1492	-0.82	5.6280	5.1492	-8.51
50	19.4800	19.4145	-0.34	18.8800	19.4145	+2.83
100	31.6700	31.7805	+0.35	33.4100	31.7805	-4.88
200	48.1400	48.0165	-0.26	50.2500	48.0165	-4.44

4 DISCUSSION

The present analysis demonstrates that expressing the CSDA mass range f(T) directly as a fifth-order polynomial in electron kinetic energy T provides a convenient semi-empirical formulation over 1–200 MeV. The parameters p_1 = 2.766×10^{-10}, p_2 = -1.616×10^{-7}, p_3 = 3.713×10^{-5}, p_4 = -0.004727, p_5 = 0.5514, and p_6 = 0.04852 explicitly define the energy-dependent behavior figure (1-2) and table (1-2) [5]. The medium-energy electron range behavior is dominated by the linear term $p_5 \cdot T$ and the non-linear curvature is provided by the higher-order terms p_1–p_4 in this equation [6]. The offset for the zero energy range p_6 is a constant. The literature of electron transport is rich with material-dependent interaction processes [14].

The meaning of the "experimental" value is an important distinction. The tabulated values in the computational database ESTAR are not measured in the laboratory, but are calculated stopping powers and ranges [1]. The numerical nature of the ESTAR calculation method is confirmed by descriptions of the calculation method [2]. In addition, independent transport-code benchmarking has been shown, such as Monte Carlo simulation toolkits (e.g. Geant4 [15]), advanced Geant4 applications (e.g. Geant4++ [16]), Monte Carlo electron-photon algorithms (e.g. GEANT4 [17]), experimental PENELOPE code benchmarks (e.g. experimental benchmarks for PENELOPE [18]), multi-code comparative study (e.g. multi-code comparative study [19]), and Monte Carlo testing codes (e.g. Monte Carlo testing codes [20]). These illustrate the independent importance of experimental benchmarking for assessing electron-transport calculations. Hence, the current comparison can be rightfully called a comparison of a semi-empirical regression with the reference calculations from ESTAR rather than a comparison with experimental measurements.

The f(T) is an empirical interpolation expression and not a fundamental transport law of the fifth order polynomial. It should be applied in the range of fitted intervals (1- 200 MeV) and should NOT be extrapolated outside this range. The quality of fit also relies on the energy grid and weighting metric chosen. The following decision is made here to avoid the domination of the objective function by the ranges with higher energies, which is why relative weighing was chosen. These computational bounds are shown by Monte Carlo code evaluations [15] [20].

The temperature and pressure used to create the water-vapor material definition is not documented in the source file. The material and gas conditions should be defined by the user and are allowed by ESTAR; therefore these should be reported in a future reproducibility record [2]. Also, without knowledge of the gas density at the conditions of interest, a geometric spread in cm-2 cannot be determined from g cm-2 [9]. The version demonstrates excessive coefficients of willpower (R^2 = zero.999981 for dry air and zero.998441 for water vapor), indicating a robust agreement between the geared up values and the reference data. Calculating the electron CSDA range in dry air and water vapor is essential for estimating electron penetration, comparing strength deposition, and expertise radiation interactions in extraordinary atmospheric conditions.

5 CONCLUSIONS

The semi-empirical polynomial $f(T) = p_1T^5 + p_2T^4 + p_3T^3 + p_4T^2 + p_5T + p_6$ provides an immediate mathematical representation of the electron CSDA mass range as a characteristic of kinetic strength T. The parameters p_1 to p_6 offer a compact analytical description over the power c program language period from 1 to 200 MeV. The version demonstrates excessive coefficients of willpower (R^2 = zero.999981 for dry air and zero.998441 for water vapor), indicating a robust agreement between the geared up values and the reference data. Calculating the electron CSDA range in dry air and water vapor is essential for estimating electron penetration, comparing strength deposition, and expertise radiation interactions in extraordinary atmospheric conditions. These calculations are mainly beneficial in radiation protection, electron beam dosimeter, atmospheric radiation delivery, and the layout of radiation detection and protecting systems. Furthermore, comparing electron levels in dry air and water vapor enables examine the have an impact on of medium composition on electron shipping and helps the development of simplified computational models.

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APPENDIX A. COMPLETE COMPARISON DATASET

The following tables contains all 37 energy points from the supplied file reproduced and fitted polynomial values and point wise relative deviations. The range values are given in g cm-2.

T (MeV)	Dry-air ESTAR	Model f(T)	Deviation (%)
1	0.4912	0.5952	+21.18
1.25	0.6408	0.7303	+13.97
1.5	0.7901	0.8647	+9.44
1.75	0.9383	0.9984	+6.41
2	1.085	1.1315	+4.29
2.5	1.374	1.3962	+1.62
3	1.658	1.6590	+0.06
3.5	1.935	1.9200	-0.78
4	2.208	2.1794	-1.29
4.5	2.476	2.4373	-1.56
5	2.74	2.6938	-1.69
5.5	2.999	2.9490	-1.67
6	3.255	3.2030	-1.60
7	3.757	3.7076	-1.31
8	4.246	4.2079	-0.90

9	4.724	4.7041	-0.42
10	5.192	5.1965	+0.09
12.5	6.323	6.4093	+1.36
15	7.405	7.5976	+2.60
17.5	8.445	8.7618	+3.75
20	9.447	9.9022	+4.82
25	11.35	12.1158	+6.75
30	13.15	14.2411	+8.30
35	14.85	16.2798	+9.63
40	16.46	18.2335	+10.77
45	18.01	20.1037	+11.63
50	19.48	21.8921	+12.38
55	20.9	23.6001	+12.92
60	22.27	25.2291	+13.29
70	24.86	28.2618	+13.68
80	27.27	31.0022	+13.69
90	29.54	33.4750	+13.32
100	31.67	35.7042	+12.74
125	36.52	40.5910	+11.15
150	40.81	44.6025	+9.29
175	44.66	47.7485	+6.92
200	48.14	50.0367	+3.94

APPENDIX B. ASSESSMENT OF THE KINETIC ENERGY EMPIRICAL PARAMETERS

The Matlab parameter set specifies $p_1 = 2.766\times10^{-10}$, $p_2 = -1.616\times10^{-7}$, $p_3 = 3.713\times10^{-5}$, $p_4 = -0.004727$, $p_5 = 0.5514$, and $p_6 = 0.04852$ for the unscaled polynomial $f(T) = p_1T^5 + p_2T^4 + p_3T^3 + p_4T^2 + p_5T + p_6$. This parameterization provides a continuous analytical function as a direct dependent expression of electron kinetic energy T.

Medium	**MAE (g cm^{-2})**	**RMSE (g cm^{-2})**	**MAPE (%)**	**Max |% error|**	**R^2**
Dry air	0.0526	0.0593	2.111	21.179	0.999981
Water vapor	0.3125	0.5433	2.806	8.931	0.998441

The explicit parameters p_1–p_6 for the dependency of kinetic energy are documented in this section and verified for both target media