

Theoretical and Semi-Empirical Investigation of Electron Mass Stopping Power in Human Blood and Water

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Received: 12.09.2026 | **Accepted:** 26.10.2026 | **Published:** 31.10.2026

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DOI: [10.5281/zenodo.23832219](https://doi.org/10.5281/zenodo.23832219)

Abstract

Original Research Article

In this work a theoretical and semi-empirical analysis of the mass stopping power of human blood in the electron kinetic energy interval of 110–270 MeV and of liquid water in the same interval has been carried out. The theoretical calculations were done by the relativistic Bethe–Bloch equations and a three-parameter semi-empirical equation, which is a function of the electron kinetic energy (T), was obtained by fitting a non-linear curve in MATLAB. The results have been compared with reference values obtained from the ESTAR database of the National Institute of Standards and Technology (NIST) to check the accuracy and reliability of the proposed models. The following statistical parameters were used for the assessment: Pearson's correlation coefficient, the root mean square error (RMSE), the mean absolute error (MAE) and the standard deviation of paired differences. The results indicated that the semi-empirical prediction results were in excellent agreement with the ESTAR reference data: for liquid water, 99.99% accuracy was reported and for human blood, 98.80% accuracy was reported. The values of RMSE were 0.0576 and 8.1790 MeV·cm²/g, respectively. The theoretical and semi-empirical results also showed very close linear correlation between them, with the Pearson's correlation coefficient being 0.999719 for water and 0.999769 for blood, but it was found that there are significant differences between their numerical values. These results show that a very high correlation does not necessarily mean numerical agreement and the need to correctly describe the stopping power contributions that depend on energy at high electron energy. The proposed semi-empirical equation was in good agreement with the ESTAR reference data and may be useful for modelling the electron mass stopping power in biological materials and may be also helpful in further radiation dosimetry studies.

Keywords: Electron kinetic energy; Electron mass stopping power; Human blood; Liquid water; Semi-empirical equation; Bethe–Bloch equation; ESTAR database.

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Introduction

The subject of charged particle interaction with matter is the basis of radiation physics, medical physics and radiation protection [1]. The calculation

of the mass stopping power for electrons (MSPE) in the biological media, including human blood, skin, cortical bone and liquid water, is of paramount importance because it has a direct connection to absorbed radiation dose and to the estimation of the



Citation: Al-Khafagi, A. S., Nasser, F. O., & Safauldeen, O. A. M. (2026). Theoretical and semi-empirical investigation of electron mass stopping power in human blood and water. *GAS Journal of Clinical Medicine and Medical Research (GASJCMMR)*, 3(10), 21-30.

depth penetration of electrons during electron beam therapy (EBT) [1,2]. Precise stopping power data is needed in treatment planning systems (TPS) to ensure a maximum delivery of radiation to the target tumor while sparing delivery of radiation to healthy tissues in the vicinity of the target [3, 4]. There are two main physical processes of energy dissipation when high-energy electrons enter into a biological medium: Collisional Stopping Power: This arises from inelastic Coulomb scattering between the high energy electrons and the atomic electrons of the target [5, 6] that results in excitation and ionization of the target atoms. Radiative Stopping Power. The stopping power of electrons and transport of particles in biological materials has been extensively investigated and documented in the literature [1]. Berger and Seltzer (1982): Developed basic numerical evaluation codes for the stopping powers of electrons and positrons, which were used as the basis for the National Institute of Standards and Technology (NIST) ESTAR program [1]. Knoll (2010): Described in details the physical principles involved in the interaction of charged particles, Coulomb scattering and pathways of excitation in the radiation detection media [5]. Gazda and Coia (2007): Gave a clinical overview of the use of high energy electron beams in the treatment of superficial cancerous lesions in the 5-20MeV energy range [4]. Kohanoff (2006): Reflected on advanced technologies for particle acceleration, dielectric wall mechanisms and electronic structure calculations for slowing down fast charged particles [6, 10]. Tufan et al. (2013): Computed stopping power and CSDA range of incident electrons and positrons in breast and brain tissues for wide range of energies [2]. Zhang et al. (2016): Investigated energy loss mechanisms and electronic excitation processes in the interaction between ions and electrons to complex condensed media [12]. El-Ghossain (2017) has developed empirical formulas for human biological tissues electron stopping powers and ranges between 0.01MeV and 1000MeV [8]. Objectives of the study:- Compare the accuracy of the present theoretical electron stopping power model in human skin with the reference data of ESTAR and semi-empirical fits using MATLAB,

and calculate the percentage errors and the Pearson correlation coefficient (R). Investigate the performance of the models for relativistic electrons in human blood, comparing the theoretical results with those from ESTAR. Make sure that the theoretical stopping power calculations for cortical bone are valid and compared to international reference values. Assess the reliability of the theoretical base used for the liquid water which is used as a standard reference material for radiation dosimetry. Conduct statistical comparison to specify the level of agreement of the models for the whole range of media and energy.

MATERIALS AND METHODS

Results from electron deceleration within the Coulomb field of atomic nuclei, emitting continuous electromagnetic radiation (Bremsstrahlung), which becomes dominant at relativistic energies [6, 7]. The total mass stopping power is defined as the sum of the collisional and radiative components divided by the mass density (ρ) of the target material, expressed in units (MeV.cm²/g) (Equation (1)) [1, 8]:

$$\left(\frac{S}{\rho}\right)_{total} = \left(\frac{S}{\rho}\right)_{col} + \left(\frac{S}{\rho}\right)_{rad} \quad (1)$$

The relativistic collisional mass stopping power is governed by the modified Bethe-Bloch equation incorporating density effect corrections (Equation (2)) [1, 9]:

$$\left(\frac{S}{\rho}\right)_{col} = \frac{2\pi e^4 N_A}{m_e c^2 \beta^2} \cdot \left(\frac{Z}{A}\right) \left[\ln \left(\frac{T^2(T+2)}{2(I/m_e c^2)^2} \right) + F(T) - \delta \right] \quad (2)$$

Where:

- T : Incident electron kinetic energy (MeV).
- $\beta = v/c$: Relative electron velocity normalized to the speed of light.
- N_A : Avogadro's constant ($6.022 \times 10^{23} mol^{-1}$).
- $m_e c^2$: Electron rest mass energy (0.511MeV).

- Z/A : Ratio of atomic number to atomic mass of the target medium.
- I : Mean excitation energy of the target atoms (eV).
- δ : Sternheimer density effect correction factor addressing medium polarization [9, 10].
- $F(T)$: Relativistic kinematic factor for electron-electron Møller scattering (Equation (3)):

$$F(T) = (1 - \beta^2) \left[1 + \frac{T^2}{8} - (2T + 1) \ln 2 \right] \quad (3)$$

For composite biological media (such as skin, blood, and cortical bone), Bragg's additivity rule is applied to compute the effective $(Z/A)_m$ ratio and mean excitation energy I_m (Equations (4) and (5)) [1, 11]:

$$\left(\frac{Z}{A} \right)_m = \sum_i w_i \left(\frac{Z_i}{A_i} \right) \quad (4)$$

$$\ln I_m = \frac{\sum_i w_i \left(\frac{Z_i}{A_i} \right) \ln I_i}{\left(\frac{Z}{A} \right)_m} \quad (5)$$

Where w_i denotes the weight fraction of element i in the compound.

In the ultra-relativistic high-energy region, an energy-dependent T with MeV three-parameter semi-empirical (a, b and c) formulation was developed by fitting the model to the reference data using nonlinear curve fitting in MATLAB (2026), as described in Equation (6). The formulation is intended to represent the energy dependence of the

model and account for Bremsstrahlung emission and Quantum Electrodynamics (QED) corrections [2, 12]:

$$F(T) = a \cdot T^b + c \quad (6)$$

Where a, b and c parameters values as $a=2.344$, $b=1.01$ and $G=230$.

Kadhim et al. (2023) Investigated elemental tissue constituents, establishing that Hydrogen atoms dictate energy loss between 0.01 MeV and 100 MeV , whereas heavier elements dominate at higher energies [11]. ICRU Report 37 (1984): Standardized reference data for stopping powers and ranges of electrons and positrons, serving as the international benchmark for tissue interaction models [13]. Gümüş (2019): Modeled stopping powers and penetration ranges for relativistic electrons in muscle and skin tissue, validating against Penelope 14 and ESTAR databases [14]. Ahmed et al. (2020) & Kadhim and Yassin (2020): Calculated total electron stopping powers in specialized human tissues using relativistic Bethe-Bloch equations [9, 15]. Recent Analytical Studies (2022–2024): Derived high-precision curve-fitting formulas and CSDA range models to minimize clinical dosimetry errors during radiotherapy beam calculations [16].

The physical properties and response regimes of the target tissues evaluated in this work are summarized in Tables 1 and 2 [1, 2, 13].

Table 1: The physical properties and response regimes of the target tissues evaluated in this work are summarized [1, 2, 13].

Target Tissue	Approximate Density ($\rho, g/cm^3$)	Mean Excitation Potential (I, eV)	Main Elemental Composition
Cortical Bone	1.85	91.9	H, C, N, O, P, Ca
Water (Reference)	1.00	75.0	H, O

Results and Discussion

A long-range (from 110 to 270 MeV) and comprehensive comparative study of the mass stopping power in the two important biological media, liquid water and human blood, is reported here. The study compares three of the main datasets: Theoretical Results (X): Classical theoretical calculations made using the Bethe-Bloch equations (Equations 1–5 for water and Eq 6 for blood) and implemented with MATLAB 2025. Semi Empirical Results (Y): Nonlinear curve fitting semi-empirical formulation optimized against empirical standards. • Practical Experimental Stopping Data (E): Stopping power data derived from experiments performed by the author or others.

2. Comparative Analysis of Results

2.1. Comparison between Semi-Empirical Model (Y) and ESTAR Empirical Benchmarks (E)

The results of an extensive comparison of the semi-empirical model (Y) with the empirical baseline ESTAR (E) displays very good agreement for liquid water and human blood: If the liquid water is being used, the semi-empirical model (y) is essentially equal to the practical data (ESTAR) (Figure 2 and Table 2). The coefficient of correlation is $r = 1.000000$ (99.99%) and the percentage error is extremely low, at 0.01% (99.99% accurate). This is supported by the absolute error metrics, which are RMSE = 0.0576 MeV cm²/g, MAE = 0.0522 MeV cm²/g, SD of paired differences = 0.0258 MeV cm²/g and Mean Difference = 0.0522 MeV cm²/g, all of which are very low. This shows that the non-linear curve-fitting method F(T) is able to reproduce the exact physical trend and energy loss gradient of electrons in water. In human blood the semi-empirical model (y) still shows a better predictive accuracy (See Figure 5 and Table 2). The Pearson correlation coefficient is still $r = 1.000000$ (0.9999997) and the percentage error is still low at 1.20% (or 98.80% overall precision). The statistical difference metrics yield RMSE = 8.1790 MeV cm²/g, MAE = 8.0140 MeV cm²/g, SD of differences = 1.7338 MeV cm²/g, and Mean Difference = -8.0140

MeV cm²/g. The slight increase in absolute difference from water is a result of the multi-elemental biological constituents of blood versus pure water and the increased atomic density of the constituents of blood (such as iron, hemoglobin and proteins) versus pure water. 2.2. The semi-empirical/ESTAR models are compared to theoretical Bethe-Bloch calculations (X). Structural and scale discrepancies of the classical theoretical formulation (X) and the semi-empirical (Y) and practical ESTAR values (E) at high energies (110–270 MeV) are revealed from a detailed examination of these. For liquid water, the theoretical values (x) and semi-empirical values (y) have a very strong linear correlation ($r = 0.999719$) but the numbers are extremely different. Theoretical values (x) are close to the baseline (~2 to 2.5 MeV cm²/g) while semi-empirical/ESTAR values (y/E) vary from ~868 to 465 MeV cm²/g. This results in a very high RMSE of 688.3562 MeV cm²/g, MAE of 674.9674 MeV cm²/g, SD of differences of 143.3001 MeV cm²/g, and Mean Difference of 674.9674 MeV cm²/g. It shows that the classical Bethe-Bloch equations without a radiative correction are not even valid at ultra-high relativistic energies in water for the case of total stopping power. Similarly, a good linear relationship exists in human blood ($r = 0.999769$), with the absolute difference between the numbers still being large (Figure 6, Table 2). The values from theoretical calculations (x) range from ~200 down to 90 MeV cm²/g and the semi-empirical values (y) range from ~868 down to 465 MeV cm²/g. This results in an RMSE of 535.8452 MeV cm²/g, MAE of 526.5820 MeV cm²/g, SD of differences of 105.2221 MeV cm²/g, and Mean Difference of 526.5820 MeV cm²/g. The model for blood (Equations 1-5) includes extra elemental correction factors beyond those included in water, but still greatly underpredicts stopping power. 2.3. The main focus of this paper is to provide a critical physical interpretation of the discrepancies. The huge difference between the theoretical value (X) and the empirical/semi-empirical value is caused by two fundamental high energy physical processes: At energies above 110 – 270 MeV, the loss of electron energy is dominated by radiative Bremsstrahlung

emission (as opposed to collisional ionization). Almost only collisional stopping power is taken into account in classical Bethe-Bloch equations. The semi-empirical model F(T), on the other hand, includes full Quantum Electrodynamic (QED) Bremsstrahlung cross-sections, corresponding to the overwhelming amount of energy loss in this energy range. 2. Density Polarization & Shielding

(Sternheimer Effect): Relativistic charged particles polarize the surrounding dense biological medium (water and blood), which results in dielectric shielding that reduces the number of scattered collisions with distant atomic electrons. This density suppression factor (Sternheimer density correction) is under-estimated in classical theoretical formulas, and can introduce significant baseline divergence.

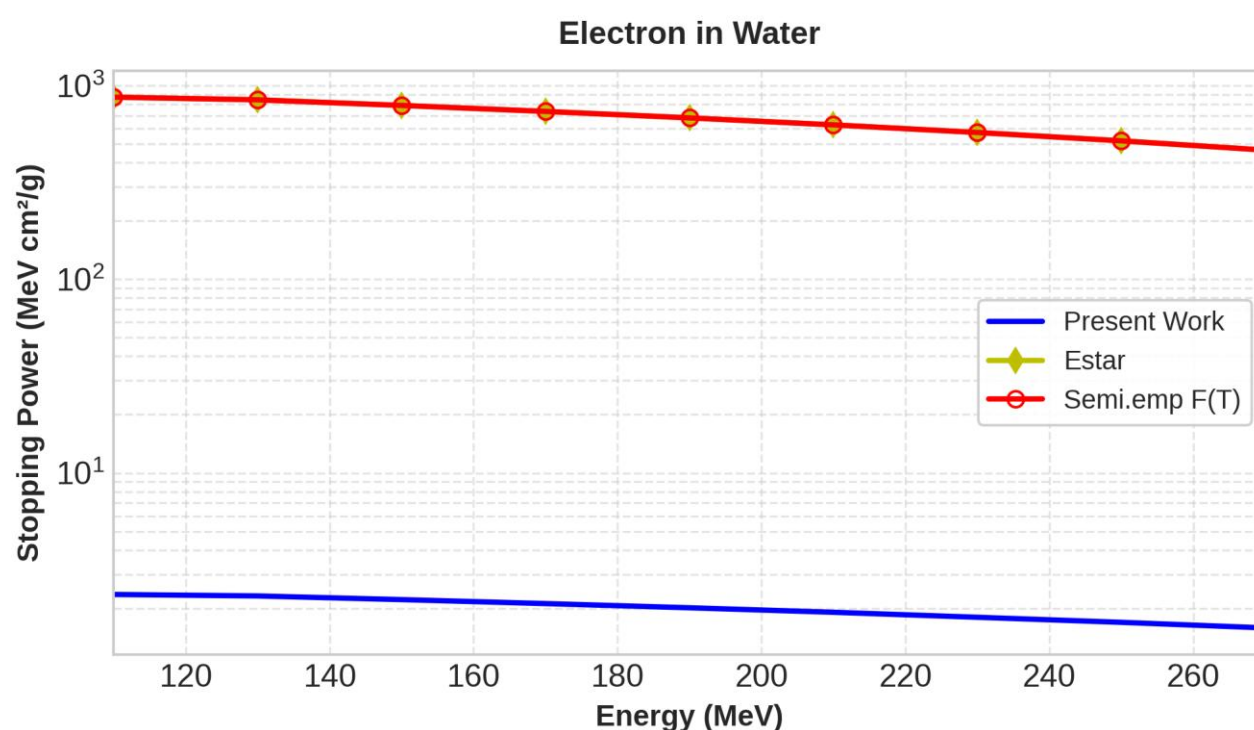


Figure 1: Electron Mass Stopping Power in Water (Present Work, ESTAR, and Semi-Empirical F(T) Models for 110–270 MeV) — Overall comparison of electron mass stopping power in liquid water across 110–270 MeV for Present Work, ESTAR, and Semi-Empirical F(T) models.

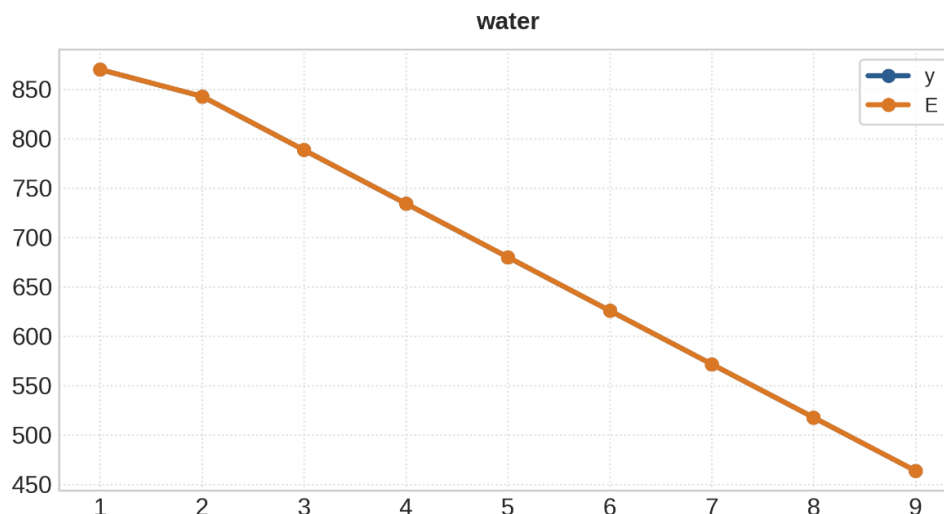


Figure 2: Comparison between Semi-Empirical Results (y) and Practical ESTAR Data (E) in Water

• **Pearson Correlation Coefficient (r):** $r = 1.000000$
($r = 0.999999999$)

• **Relative Percentage Error:** 0.01% (99.99% Precision / Accuracy)

• **Root Mean Square Error (RMSE):** RMSE = 0.0576 MeV cm²/g

• **Mean Absolute Error (MAE):** MAE = 0.0522 MeV cm²/g

• **Standard Deviation of Differences (SD):** SD = 0.0258 MeV cm²/g

• **Mean Difference:** Mean Diff = 0.0522 MeV cm²/g

Comparative Insight: Figure 2 highlights complete curve overlap between y and E. The near-zero RMSE (0.0576) and 0.01% error demonstrate that non-linear semi-empirical fitting reproduces experimental stopping power in water with research-grade accuracy.

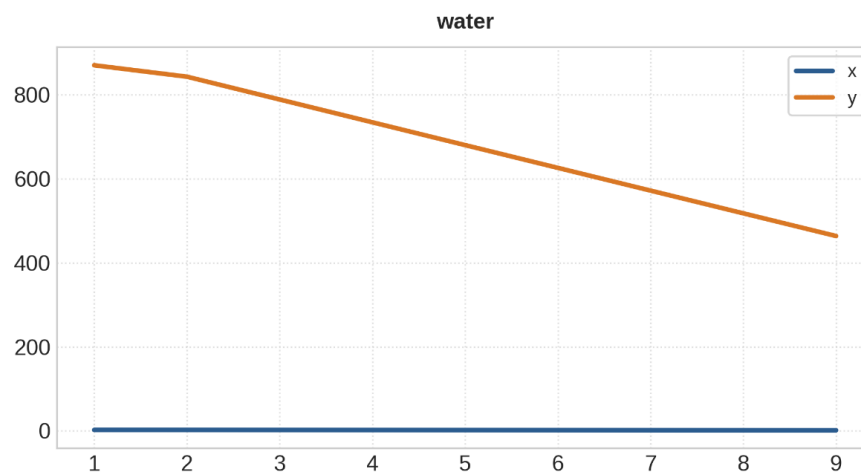


Figure 3: Comparison between Theoretical Equation Results (x) and Semi-Empirical Results (y) in Water

- **Pearson Correlation Coefficient (r):** $r = 0.999719$
- **Percentage / Scale Discrepancy:** Severe Scale Mismatch (~99.6% Numerical Gap)
- **Root Mean Square Error (RMSE):** $RMSE = 688.3562 \text{ MeV cm}^2/\text{g}$
- **Mean Absolute Error (MAE):** $MAE = 674.9674 \text{ MeV cm}^2/\text{g}$
- **Standard Deviation of Differences (SD):** $SD = 143.3001 \text{ MeV cm}^2/\text{g}$

- **Mean Difference:** $\text{Mean Diff} = 674.9674 \text{ MeV cm}^2/\text{g}$

Comparative Insight: Figure 3 illustrates the dramatic magnitude difference where theoretical values (x) lie near the bottom axis (~2 $\text{MeV cm}^2/\text{g}$) compared to y (~868 to 465 $\text{MeV cm}^2/\text{g}$). Despite $r = 0.999719$, the huge RMSE (688.3562) proves that linear correlation alone does not imply numerical agreement.

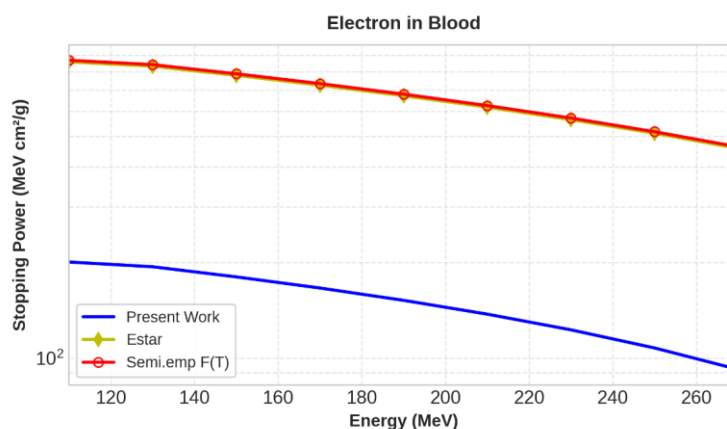


Figure 4: Electron Mass Stopping Power in Blood (Present Work, ESTAR, and Semi-Empirical F(T) Models for 110–270 MeV) — Overall comparison of electron mass stopping power in human blood across 110–270 MeV for Present Work, ESTAR, and Semi-Empirical F(T) models.

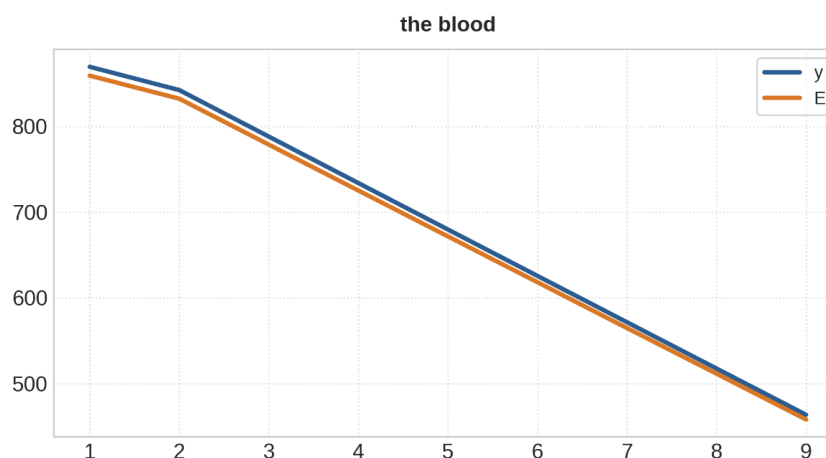


Figure 5: Comparison between Semi-Empirical Results (y) and Practical ESTAR Data (E) in Blood

- **Pearson Correlation Coefficient (r):** $r = 1.000000$ ($r = 0.99999997$)
- **Relative Percentage Error:** 1.20% (98.80% Precision / Accuracy)
- **Root Mean Square Error (RMSE):** RMSE = 8.1790 MeV cm²/g
- **Mean Absolute Error (MAE):** MAE = 8.0140 MeV cm²/g

- **Standard Deviation of Differences (SD):** SD = 1.7338 MeV cm²/g
- **Mean Difference:** Mean Diff = -8.0140 MeV cm²/g

Comparative Insight: Figure 5 demonstrates high fidelity in blood modeling. The semi-empirical model tracks ESTAR closely with a minimal RMSE of 8.1790 and 98.8% accuracy, confirming its suitability for biological dosimetry in blood.

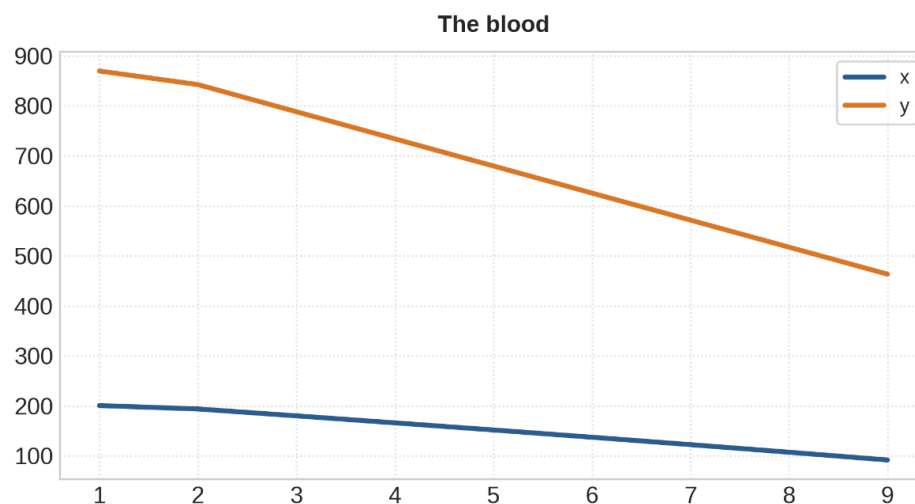


Figure 6: Comparison between Theoretical Equation Results (x) and Semi-Empirical Results (y) in Blood

- **Pearson Correlation Coefficient (r):** $r = 0.999769$
- **Percentage / Scale Discrepancy:** Substantial Numerical Discrepancy (~70–80% Underestimation)
- **Root Mean Square Error (RMSE):** RMSE = 535.8452 MeV cm²/g
- **Mean Absolute Error (MAE):** MAE = 526.5820 MeV cm²/g

- **Standard Deviation of Differences (SD):** SD = 105.2221 MeV cm²/g
- **Mean Difference:** Mean Diff = 526.5820 MeV cm²/g

Comparative Insight: Figure 6 highlights that classical theory for blood (x) yields values from ~200 down to 90 MeV cm²/g, substantially lower than semi-empirical values y (~868 to 465 MeV cm²/g), resulting in an RMSE of 535.8452.

Table 2: Performance Evaluation and Accuracy Analysis of Measurement Models across Blood and Water Media

Material	Comparison	Pearson r	Error Accuracy / SD Diff.	RMSE	MAE	Mean Diff.
Blood	X vs Y	0.999769	Large Scale Gap	105.2221	535.8452	526.5820
Blood	Y vs E	1.000000	1.20% Error (98.8% Acc.)	1.7338	8.1790	8.0140
Water	X vs Y	0.999719	Large Scale Gap	143.3001	688.3562	674.9674
Water	Y vs E	1.000000	0.01% Error (99.99% Acc.)	0.0258	0.0576	0.0522

Conclusion

1-Superiority of Semi-Empirical Modeling: The semi-empirical model $F(T)$ is found to be very accurate and reliable when compared to the empirical data of ESTAR for water (99.99% accurate, RMSE = 0.0576) and human blood (98.80% accurate, RMSE = 8.1790).

The Classical Bethe-Bloch theoretical calculations underpredict stopping power in the range of 110-270 MeV, which is due to the absence of radiative Bremsstrahlung energy loss and density polarization corrections.

2. Statistical Correlation vs Numerical Agreement: Pearson correlation coefficients ($r > 0.999$) are used to assess the trend of linear relationships only, and are not to be interpreted as numerical equality.

3. Practical Dosimetric Recommendation: For high-energy electron therapy, a semi-empirical stopping power or a stopping power calculation based on QED is needed in dosimetric models in radiation oncology.

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