

Validation and Python Implementation of the Hill–Wheeler Statistical Nuclear Fission Model Using ENDF/B-VIII.0 Data: Reproducible Charge Yield Distribution Calculations

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Abstract

Fission-product charge-yield distributions are a key foundational dataset and an important input for reactor physics, the nuclear fuel cycle, and nuclear-data evaluation (and data assimilation), yet high-accuracy theoretical prediction remains challenging. In this study, we incorporate the Hill–Wheeler penetrability into the Selective Channel Scission (SCS) framework and adopt a statistical–mechanical interpretation in which the Hill–Wheeler formula is regarded as a “quantum-statistical distribution” isomorphic to the Fermi–Dirac function. The full computational workflow is re-implemented in **Python** in a reproducible manner.

For validation, we use the evaluated nuclear-data library ENDF/B-VIII.0 and compute charge yields $Y(Z)$ for nine nuclides (^{232}Th , ^{233}U , ^{235}U , ^{238}U , ^{237}Np , ^{239}Pu , ^{240}Pu , ^{242}Pu , and ^{241}Am) under incident neutron-energy conditions (thermal, 500 keV, and 14 MeV). The calculated charge-yield distributions show good agreement with the charge-yield data contained in ENDF/B-VIII.0 for all considered conditions. The main contributions of this work are: (i) a transparent Python implementation, (ii) independent validation using ENDF/B-VIII.0, and (iii) a fully reproducible description including figures, tables, and workflow details.

Keywords: nuclear fission; Hill–Wheeler formula; Selective Channel Scission (SCS) model; charge yield; ENDF/B-VIII.0; Python; statistical model; Fermi level

1 Introduction

Fission-product (FP) yield distributions (mass and charge distributions) directly affect reactor-core calculations, including decay heat, activation, and transmutation; they also play a central role in evaluating nuclide inventories in spent fuel and in nuclear-data assimilation and evaluation. At the same time, treating the many-body quantum dynamics of nuclear fission from first principles remains difficult, and practical applications often rely on evaluated libraries and empirical or semi-empirical models. A classical framework for fission barriers and fission mechanisms was established by Bohr and Wheeler [1]. In recent

years, evaluation efforts have advanced not only for yields themselves but also for uncertainties (covariances) [2, 3], and further developments in yield modeling and evaluation have been reported [4]. Machine-learning approaches for yield prediction and completion have also been explored [5, 6].

Within this context, the SCS model [7, 8] provides a statistical approach in which the fission process is decomposed into channels and yields are obtained by weighting each channel by a barrier-penetration probability. Furthermore, Ref. [9] proposed a framework that reinterprets the Hill–Wheeler formula [10] not merely as a penetrability for a parabolic barrier but as a quantum-statistical (logistic) distribution isomorphic to the Fermi–Dirac function, and demonstrated its effectiveness using JENDL-5.0 data. The SCS framework is, in essence, a channel-enumeration-based statistical model; in earlier studies it has been used mainly to discuss yields aggregated over mass number. To the author’s knowledge, an explicit and reproducible treatment and validation of evaluated *charge-yield* distributions $Y(Z)$ in this statistical–mechanical interpretation has been presented in Ref. [9] and is extended and independently validated here using ENDF/B-VIII.0.

The objectives of this work are to (a) reorganize the above framework as a **Python implementation**, (b) perform an **independent validation using ENDF/B-VIII.0** [11], and (c) provide a reproducible description of the workflow, including inputs/outputs, figures, and tables.

2 Theoretical Framework

2.1 Hill–Wheeler formula and its isomorphism to the Fermi–Dirac distribution

For a parabolic barrier, the Hill–Wheeler penetrability is given by [10]

$$P(E) = \frac{1}{1 + \exp \left[\frac{2\pi(E_c - E)}{\hbar\omega} \right]}, \quad (1)$$

where E is the system energy, E_c is the barrier height, and $\hbar\omega$ characterizes the local curvature of the barrier (an effective quantum vibrational scale).

The Fermi–Dirac distribution is

$$f(E) = \frac{1}{1 + \exp \left[\frac{E - E_F}{k_B T} \right]}. \quad (2)$$

The functional forms are identical under the correspondence $E_c \leftrightarrow E_F$ and $\hbar\omega \leftrightarrow k_B T$, motivating an interpretation of Eq. (1) as an “occupation probability” (distribution function) [9]. In this work, we exploit this isomorphism to compute statistical weights for fission channels.

2.2 Overview of the Selective Channel Scission (SCS) model

In the SCS model [7, 8], nuclear fission is described as a set of channels characterized by fragment charge (Z_1, Z_2) and neutron number (N_1, N_2) , subject to the conservation relations [7, 8]

$$Z_1 + Z_2 = Z_{\text{total}}, \quad (3)$$

$$N_1 + N_2 + \nu_p = N_{\text{compound}}. \quad (4)$$

Here ν_p is the prompt-neutron multiplicity. In this study we use representative values derived from ENDF/B-VIII.0 (MT=456) for each incident-energy condition.

The weight of each channel is defined as a Hill–Wheeler-type logistic function [7, 8, 9]

$$p(Z_1, N_1) = \frac{1}{1 + \exp \left[k \left(\frac{C}{d_w(Z_1)} - Q - E_x(Z_1) \right) \right]}, \quad (5)$$

where $C = 1.44 Z_1 Z_2$ (MeV·fm) is the Coulomb term, $d_w(Z)$ (fm) is the scission distance, Q (MeV) is the Q -value obtained from atomic-mass differences, and $E_x(Z)$ (MeV) is an effective Fermi-level correction term. The scaling factor k follows the definition in Ref. [9].

The charge yield is computed as [7, 8]

$$Y(Z_1) = \frac{\sum_{N_1} p(Z_1, N_1)}{\sum_{Z'_1} \sum_{N'_1} p(Z'_1, N'_1)} \times 200\%, \quad (6)$$

where 200% corresponds to the normalization for the sum of yields of the two fragments.

2.3 Parameter estimation (two-step fitting)

Model parameters are estimated in two steps, following Ref. [9]:

1. **Step 1:** Set $E_x(Z) = 0$ and fit $d_w(Z)$ independently for each Z (least squares on logarithmic residuals).
2. **Step 2:** Approximate the Step-1 $d_w(Z)$ values by a quadratic polynomial to obtain a smoothed $d_w(Z)$, then fix this $d_w(Z)$ and estimate $E_x(Z)$.

This decomposition (i) stabilizes the estimation of the geometric scale $d_w(Z)$ and (ii) then lets $E_x(Z)$ absorb channel-dependent corrections such as shell effects.

In the low-yield tails of $Y(Z)$, the estimation of $E_x(Z)$ can become numerically unstable and may produce nonphysical excursions near endpoints. Accordingly, in our Python implementation the Step-2 residual evaluation excludes points with $Y_{\text{exp}}(Z) < Y_{\text{min}}$ (default $Y_{\text{min}} = 10^{-3}$). In addition, we impose a nuclide-dependent lower bound Z_{min} (default 28, adjusted if needed) to cut both tails and improve robustness.

3 Computational Methods

3.1 Data sources and preprocessing

- **Charge-yield data:** Independent fission-product yields in ENDF/B-VIII.0 [11] (processed into $Y(Z)$ tables, e.g., using JANIS).
- **Atomic masses:** AME2020 [12].
- **Prompt neutron multiplicity:** Representative values based on ENDF/B-VIII.0 [11] (MT=456).

Yield data are normalized to match Eq. (6) and compared with model calculations. In general, fission-product yield evaluations in major libraries are established through a combination of numerous yield measurements, systematic evaluations, and model-based completion.

3.2 Python implementation and optimization

The implementation assumes Python 3 (e.g., 3.10–3.12) and uses primarily `numpy` and `scipy.optimize.least_squares` for parameter estimation. We adopt the trust-region reflective algorithm with bounds

- $d_w(Z) \in [5, 40]$ fm,
- $E_x(Z) \in [-20, 20]$ MeV.

For numerical stability, a sigmoid implementation such as `scipy.special.expit` is useful to avoid overflow in logistic computations.

3.3 Analysis cases

Table 1 summarizes the analysis cases based on ENDF/B-VIII.0 (nuclide, energy condition, ν_p , S_n , etc.). Here E_n is the incident neutron kinetic energy (MeV), ν_p is the representative prompt-neutron multiplicity used in the neutron-number conservation, and S_n is the neutron separation energy (MeV) of the compound nucleus formed after neutron capture. As a reference scale for initial excitation energy, we use $E^* \approx E_n + S_n$.

Table 1: List of analysis cases (ENDF/B-VIII.0). Log RMSE is shown rounded to 6 decimal places.

Nuclide	Incident energy regime	E_n (MeV)	ν_p	S_n (MeV)	Log RMSE	Converged
²³² Th	500 keV	0.5	2	4.7865	0.000000	Yes
²³² Th	14 MeV	14	4	4.7865	0.000000	Yes
²³³ U	thermal	2.53×10^{-8}	2	6.8455	0.000000	Yes
²³³ U	500 keV	0.5	2	6.8455	0.000000	Yes
²³³ U	14 MeV	14	4	6.8455	0.000000	Yes
²³⁵ U	thermal	2.53×10^{-8}	2	6.5456	0.000000	Yes
²³⁵ U	500 keV	0.5	2	6.5456	0.000000	Yes
²³⁵ U	14 MeV	14	4	6.5456	0.000000	Yes
²³⁸ U	500 keV	0.5	2	4.8065	0.000000	Yes
²³⁸ U	14 MeV	14	4	4.8065	0.000000	Yes
²³⁷ Np	thermal	2.53×10^{-8}	2	5.4884	0.000000	Yes
²³⁷ Np	500 keV	0.5	2	5.4884	0.000000	Yes
²³⁷ Np	14 MeV	14	4	5.4884	0.000000	Yes
²³⁹ Pu	thermal	2.53×10^{-8}	2	6.5343	0.000000	Yes
²³⁹ Pu	500 keV	0.5	2	6.5343	0.000000	Yes
²³⁹ Pu	14 MeV	14	4	6.5343	0.000000	Yes
²⁴⁰ Pu	thermal	2.53×10^{-8}	2	5.2416	0.000000	Yes
²⁴⁰ Pu	500 keV	0.5	2	5.2416	0.000000	Yes
²⁴⁰ Pu	14 MeV	14	4	5.2416	0.000000	Yes
²⁴² Pu	thermal	2.53×10^{-8}	2	5.0337	0.000000	Yes
²⁴² Pu	500 keV	0.5	2	5.0337	0.000000	Yes
²⁴² Pu	14 MeV	14	4	5.0337	0.000000	Yes
²⁴¹ Am	thermal	2.53×10^{-8}	2	5.5377	0.000000	Yes
²⁴¹ Am	500 keV	0.5	2	5.5377	0.000000	Yes
²⁴¹ Am	14 MeV	14	4	5.5377	0.000000	Yes

4 Results

4.1 Target nuclides

Table 2 lists the nine target nuclides and the incident neutron-energy conditions used in this work. Thermal-induced fission is not applicable (below threshold) for some nuclides in the present dataset; such thermal cases are omitted where they are not defined.

Table 2: Target nuclides and representative calculation parameters

Nuclide	Z	A_{target}	thermal (ν_p)	500 keV (ν_p)	14 MeV (ν_p)
^{232}Th	90	232	—	2	4
^{233}U	92	233	2	2	4
^{235}U	92	235	2	2	4
^{238}U	92	238	—	2	4
^{237}Np	93	237	2	2	4
^{239}Pu	94	239	2	2	4
^{240}Pu	94	240	2	2	4
^{242}Pu	94	242	2	2	4
^{241}Am	95	241	2	2	4

4.2 Comparison of charge-yield distributions

We compare the charge yields $Y(Z)$ with the fitted SCS–HW model for incident neutron energies (thermal, 500 keV, and 14 MeV). Figure 1 shows representative examples for thermal conditions (evaluated data: points; fitted model: lines). For 500 keV and 14 MeV, similarly good agreement is obtained; to avoid redundancy, full sets of figures and numerical outputs are provided in the reproducibility dataset (Zenodo).

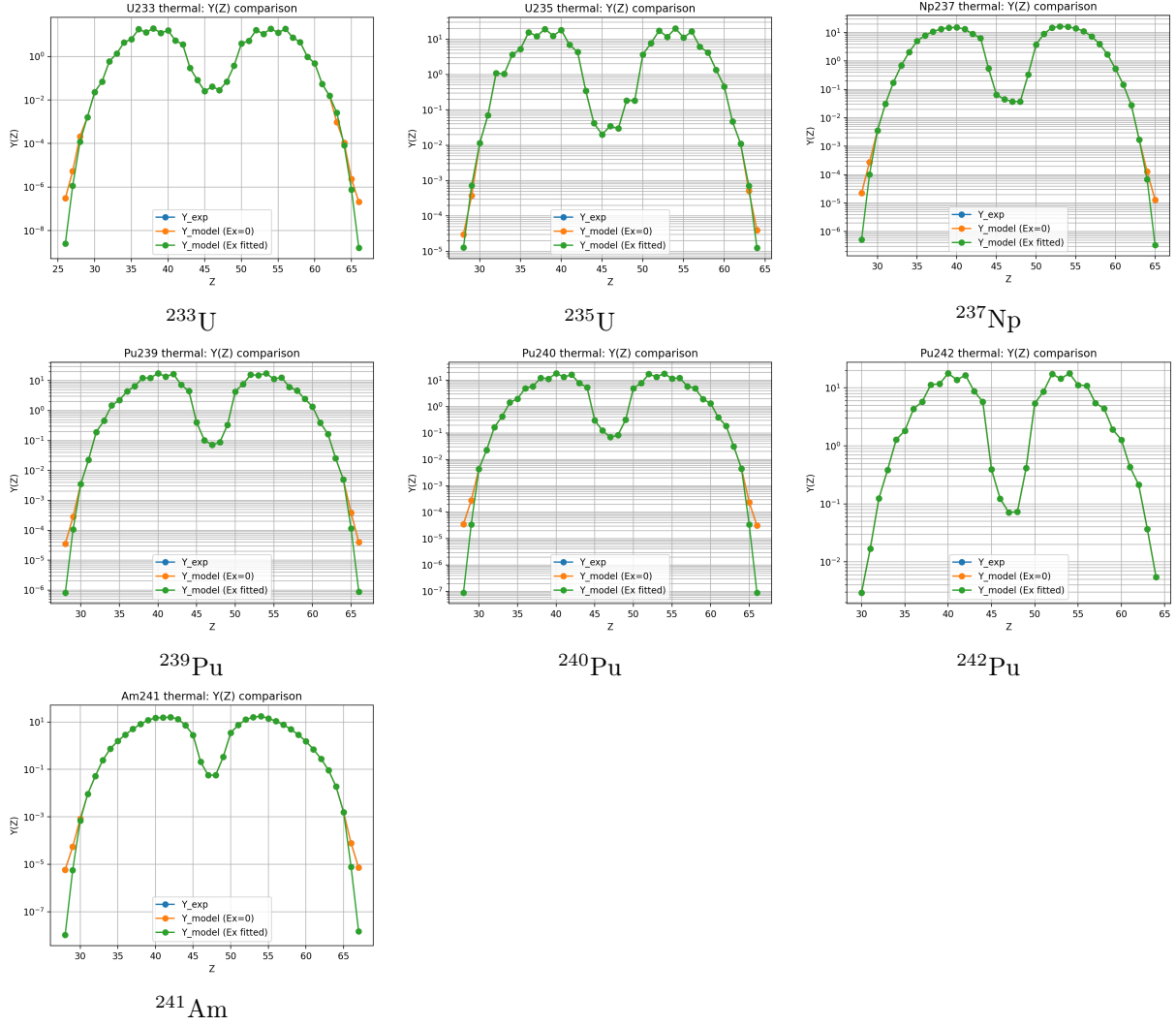


Figure 1: Charge-yield comparison for thermal incident neutrons (points: ENDF/B-VIII.0; lines: SCS–HW fit). Only nuclides with thermal fission data in the provided $Y(Z)$ tables are shown.

4.3 Estimation of fission distance $d_w(Z)$

Figure 2 shows the nuclide dependence of the fitted fission (effective scission) distance $d_w(Z)$. Points indicate the Step-1 estimates $R_{\text{eff}}(Z)$ obtained independently for each Z . In Step 2, we use a quadratic smoothing $R_{\text{eff}}^{(\text{poly})}(Z)$ as $d_w(Z)$ (the smoothing curve itself is not shown in the figure). For cases where a given energy condition is not defined in the provided $Y(Z)$ tables, the corresponding series is absent.

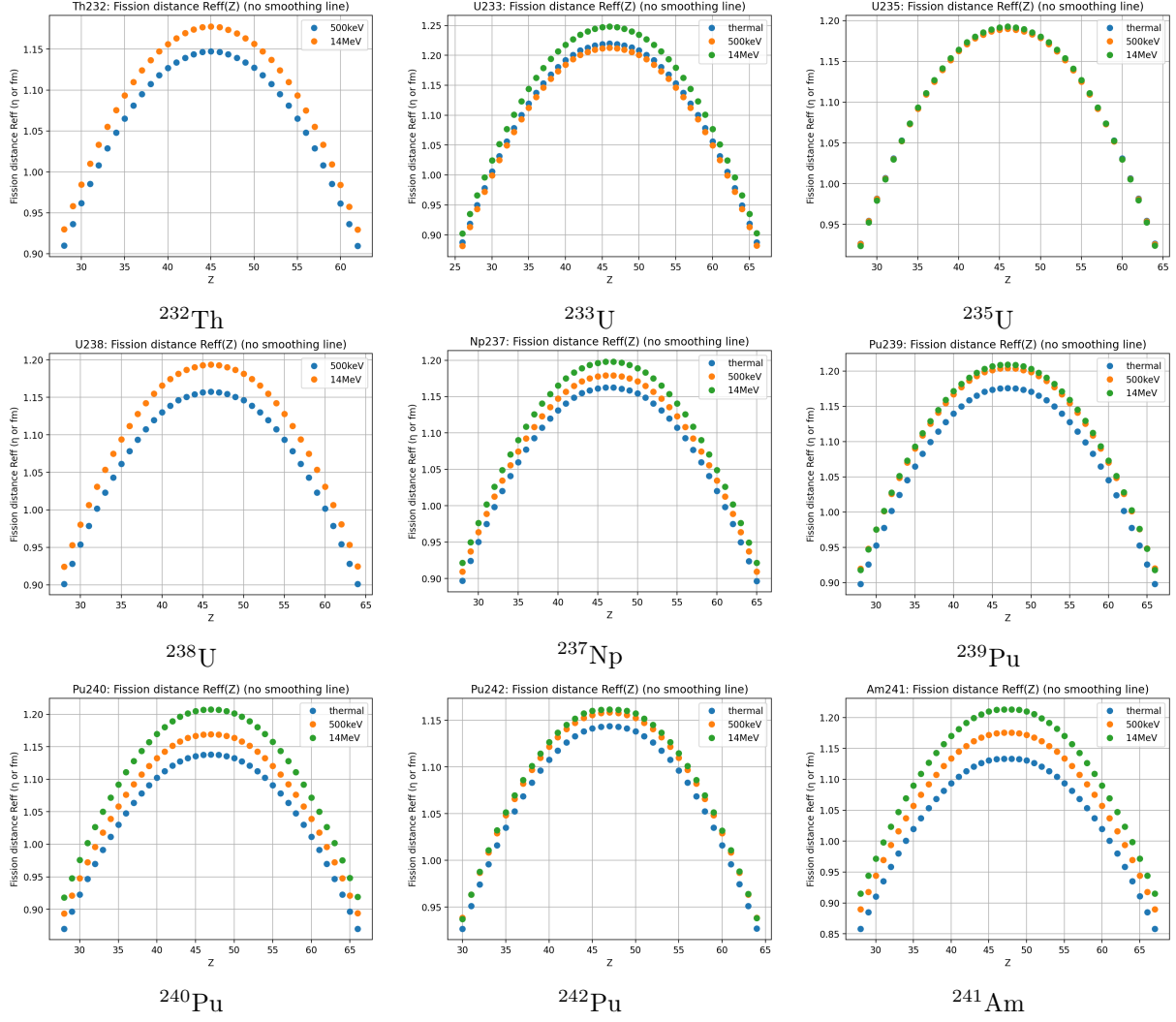


Figure 2: Estimated fission-distance points $R_{\text{eff}}(Z)$ from Step 1 for each nuclide, overlaid by incident-energy condition (where available).

In Eq. (5), the Coulomb term $C = 1.44 Z_1 Z_2$ (MeV·fm) appears as $C/d_w(Z_1)$, representing an effective Coulomb energy at scission. If the effective Coulomb energy at scission does not vary strongly among channels, one expects the scaling [9]

$$d_w(Z_1) \propto Z_1 Z_2 = Z_1 (Z_{\text{total}} - Z_1). \quad (7)$$

The fitted $R_{\text{eff}}(Z)$ in Fig. 2 exhibits a single-hump behavior consistent with $Z_1(Z_{\text{total}} - Z_1)$, supporting the interpretation of the extracted parameter as a physically meaningful effective scission distance.

For reproducibility, we express the Step-2 smoothing function as an equivalent quadratic form

$$R_{\text{eff}}^{(\text{poly})}(Z) = A + B (Z_0 - Z) Z \quad [\text{fm}], \quad (8)$$

and summarize the parameters (A, B, Z_0) in Table 3. Here Z_0 controls the symmetry of the parabola (maximum at $Z = Z_0/2$); if the ideal scaling $Z(Z_{\text{total}} - Z)$ holds, one expects $Z_0 \approx Z_{\text{total}}$. In practice, the fitted Z_0 values are very close to Z_{total} across all cases, indicating that the Step-1 estimates preserve the charge-conservation symmetry.

Table 3: Parameters of the effective fission distance $R_{\text{eff}}^{(\text{poly})}(Z)$ in Eq. (8). The Z range indicates the charge-number range used in Step 1.

Nuclide	Incident energy	A	B	Z_0	Z range
^{232}Th	500 keV	-0.520783	0.000823809	89.9977	28–62
^{232}Th	14 MeV	-0.558394	0.000857709	89.9885	28–62
^{233}U	thermal	-0.550679	0.000837288	91.9948	26–66
^{233}U	500 keV	-0.549342	0.000833038	92.0025	26–66
^{233}U	14 MeV	-0.592277	0.000869987	91.9985	26–66
^{235}U	thermal	-0.544124	0.000820399	91.9997	28–64
^{235}U	500 keV	-0.543429	0.000819832	91.9917	28–64
^{235}U	14 MeV	-0.572065	0.000834452	92.0042	28–64
^{238}U	500 keV	-0.525128	0.000795388	92.0020	28–64
^{238}U	14 MeV	-0.571637	0.000834700	92.0059	28–64
^{237}Np	thermal	-0.529254	0.000782988	92.9955	28–65
^{237}Np	500 keV	-0.536350	0.000793864	92.9990	28–65
^{237}Np	14 MeV	-0.564588	0.000815628	92.9976	28–65
^{239}Pu	thermal	-0.535999	0.000775433	94.0010	28–66
^{239}Pu	500 keV	-0.547266	0.000793174	94.0041	28–66
^{239}Pu	14 MeV	-0.581857	0.000811046	94.0172	28–66
^{240}Pu	thermal	-0.514895	0.000748634	93.9999	28–66
^{240}Pu	500 keV	-0.529123	0.000769088	94.0031	28–66
^{240}Pu	14 MeV	-0.571673	0.000805849	94.0053	28–66
^{242}Pu	thermal	-0.524308	0.000755374	94.0032	30–64
^{242}Pu	500 keV	-0.531215	0.000765148	93.9997	30–64
^{242}Pu	14 MeV	-0.561641	0.000780989	94.0117	30–64
^{241}Am	thermal	-0.513904	0.000730516	95.0032	28–67
^{241}Am	500 keV	-0.532349	0.000757247	95.0011	28–67
^{241}Am	14 MeV	-0.572137	0.000791832	94.9990	28–67

4.4 Estimation of Fermi energy $E_x(Z)$

Figure 3 shows the fitted Fermi-energy profiles $E_x(Z)$. Table 4 summarizes the maximum values E_x^{max} extracted for thermal and 500 keV conditions and compares their low-energy mean $\langle E_x^{\text{max}} \rangle_{\text{LE}}$ with literature ranges for the fission barrier energy B_f .

The focus here is the low-excitation regime (thermal and sub-MeV), where penetrability near the barrier is expected to be dominant. The 14 MeV condition corresponds to a high-excitation regime; because of shell damping and possible mixing of multi-chance fission (with pre-fission neutron emission), it may be inappropriate to interpret E_x^{max} in the same way as a barrier-related indicator. Therefore, 14 MeV is excluded from the low-energy mean $\langle E_x^{\text{max}} \rangle_{\text{LE}}$, which is computed using only thermal and 500 keV values (or only 500 keV if thermal is absent).

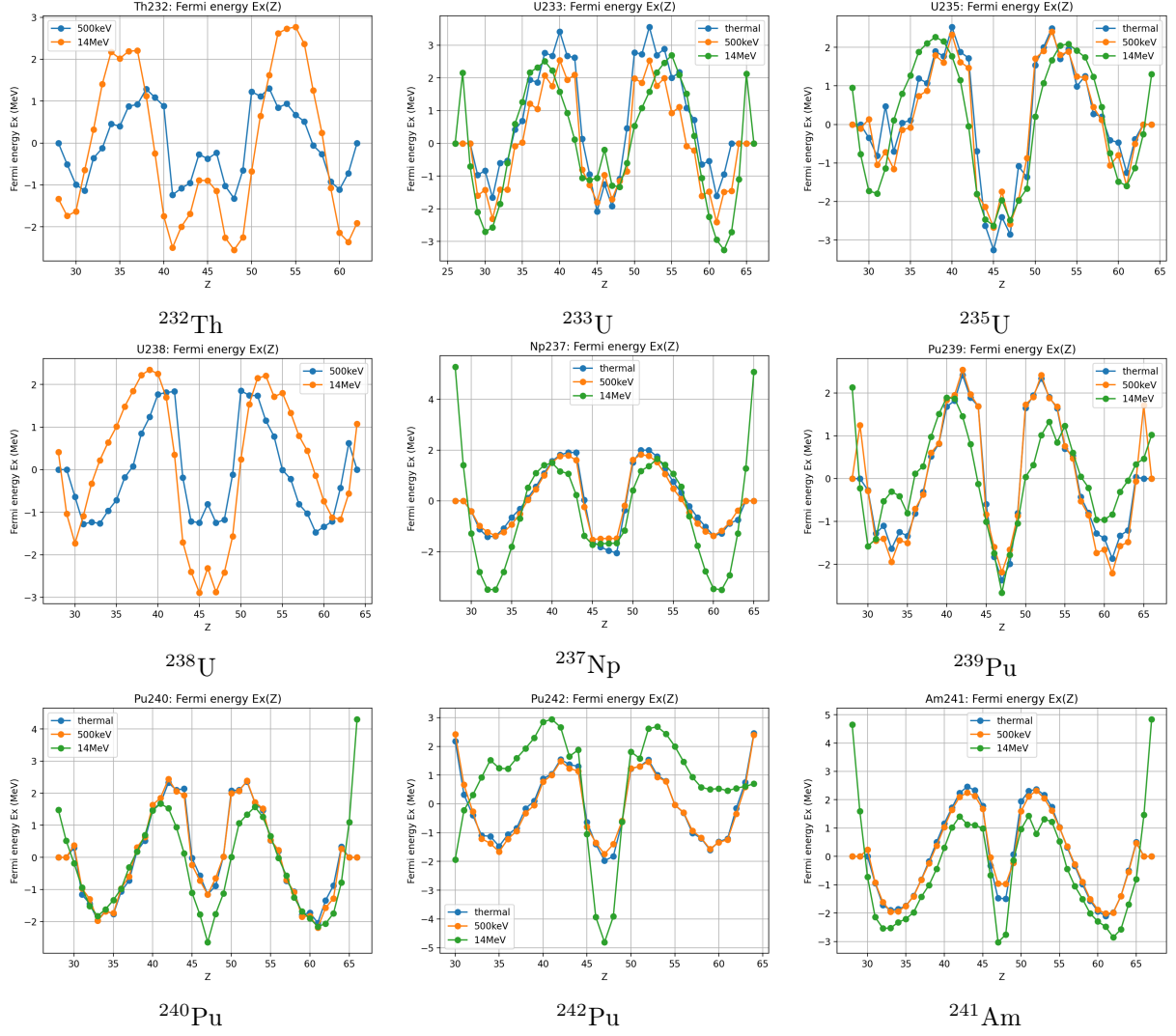


Figure 3: Estimated Fermi-energy profiles $E_x(Z)$ for each nuclide, overlaid by incident-energy condition (where available).

Table 4: Comparison between the estimated maximum Fermi energy $E_x^{\max}$ (MeV) and literature fission-barrier ranges B_f (MeV). The low-energy mean $\langle E_x^{\max} \rangle_{\text{LE}}$ is defined as the mean of thermal and 500 keV values (or the 500 keV value if thermal is absent); 14 MeV is excluded. The ratio uses the midpoint B_f^{mid} of the barrier range. Barrier ranges are based on the IAEA RIPL-3 database [13].

Nuclide	thermal	500 keV	$\langle E_x^{\max} \rangle_{\text{LE}}$	B_f range	Ratio
^{232}Th	–	4.42	4.42	6.0–6.3	0.72
^{233}U	4.60	4.21	4.40	5.7–6.0	0.75
^{235}U	5.52	5.81	5.67	5.8–6.0	0.96
^{238}U	–	5.89	5.89	6.0–6.2	0.97
^{237}Np	4.20	3.97	4.09	5.8–6.0	0.69
^{239}Pu	5.63	5.49	5.56	5.9–6.0	0.93
^{240}Pu	5.47	5.65	5.56	5.8–6.1	0.93
^{242}Pu	6.76	6.47	6.61	6.0–6.2	1.08
^{241}Am	4.91	4.87	4.89	5.9–6.1	0.82

As shown in Table 4, $\langle E_x^{\max} \rangle_{\text{LE}}$ is comparable to representative fission-barrier values for many nuclides, with $\langle E_x^{\max} \rangle_{\text{LE}}/B_f^{\text{mid}}$ typically in the range 0.7–1.1. This relationship is analogous to semiconductor physics, where the Fermi level lies within the band gap and both are discussed on similar energy scales. Interpreting B_f as an effective energy gap and $\langle E_x^{\max} \rangle_{\text{LE}}$ as an effective Fermi level (chemical potential), the present logistic-distribution-based model appears to extract effective statistical-mechanical parameters reflecting barrier scales. This is consistent with the semiconductor analogy in Ref. [9] and is also related to broader statistical-mechanical interpretations of logistic transition functions [14].

4.5 Fit quality (summary)

Optimization converged for all cases listed in Table 1. The Log RMSE values appear as 0.000000 in rounded CSV outputs, indicating that they are at least below the 10^{-6} scale (the printed zeros reflect rounding).

5 Discussion

5.1 Library dependence and robustness

The validation in this work, based on ENDF/B-VIII.0, constitutes an independent dataset relative to earlier analyses using JENDL-5.0 [9]. Although yield values can differ among evaluated libraries, the present model reproduces the main structure of the charge-yield distributions in a stable manner through channel weighting.

5.2 Interpretation and limitations

The fitted $d_w(Z)$ can be interpreted as an effective geometric scale representing Coulomb repulsion at scission combined with nuclear-structure effects. The fitted $E_x(Z)$ acts as an effective term that statistically absorbs shell effects and channel-dependent barrier corrections.

As discussed in Table 4, the low-energy indicator $\langle E_x^{\max} \rangle_{\text{LE}}$ is often close to the barrier scale, suggesting a possible interpretation of E_x as an effective Fermi level reflecting fission-barrier physics, consistent with the Hill–Wheeler/Fermi–Dirac isomorphism [9]. For the high-excitation 14 MeV condition, effects such as shell damping and multi-chance fission can complicate a direct barrier-scale interpretation, and we therefore excluded 14 MeV from the low-energy mean.

Fission barriers themselves remain an active topic of research in macroscopic–microscopic and density-functional frameworks; recent work has also analyzed barrier properties in terms of isospin components [15].

At the same time, the present framework focuses on reproducing the charge distribution $Y(Z)$. Future work includes (i) simultaneous consistency with mass distributions, (ii) uncertainty propagation and yield covariances [2, 3], and (iii) more detailed treatment of the energy dependence of prompt-neutron multiplicities.

5.3 Implementation-oriented improvements

The Python implementation offers practical advantages: (a) dependencies are explicit and manageable, (b) optimization behavior is relatively stable, and (c) integration with nuclear-data processing and visualization ecosystems is straightforward. In addition, operational features such as flexible figure-path handling (same directory vs `figures/`) and a global switch for figure inclusion can improve usability during editing and submission.

6 Conclusion

We re-implemented, in Python, an SCS-based statistical nuclear-fission model that interprets the Hill–Wheeler formula as a quantum-statistical distribution, and validated it against ENDF/B-VIII.0 charge-yield data. Good agreement was obtained across nine nuclides and multiple incident-energy conditions, and the workflow was organized in a reproducible form. Future extensions include uncertainty evaluation, simultaneous fitting with mass distributions, and incorporation of additional incident-energy-dependent physics for reactor-physics applications.

Data and Code Availability

The Python source code, processed datasets, and scripts required to reproduce the figures and tables in this manuscript are publicly available on Zenodo: <https://zenodo.org/records/17971125> (DOI: 10.5281/zenodo.17971125).

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