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ABSTRACT

Average cross-sections are calculated, with the NJOY code, for some reactions of the ENDF/B-V dosimetry file, with a view to comparing them with the experimental values. The Watt and Madland-Nix representations for the ^{235}U and ^{252}Cf fission spectra are used as the weighting functions. The STAY'SL code is used to adjust these spectra and new values for the average cross-sections are obtained using the adjusted spectra.

1. INTRODUCTION

The reproduction of experimental values for average cross-sections by means of various representations of the fission spectrum for heavy elements has been under study for more than a decade. The most suitable form for the analytical description of fission spectra is the subject under investigation. The first approximation used, the Maxwellian form [1], is a function of only one parameter; subsequently, the Watt formula [1] included a function of two parameters. A more recent representation for describing the fission spectrum, proposed by Madland and Nix [2], includes a dependence on three parameters.

The objective of the present study is the calculation of average cross-sections (for one energy group), weighted by the fission spectra for ^{235}U and ^{252}U given by the Watt and the Madland-Nix representations. These values are compared with the experimental data. An adjustment was also made to the theoretical spectra by means of experimental data (spectrum unfolding) through the use of the STAY'SL program [3]. The values for the average cross-sections are recalculated by the use of the adjusted spectra and compared again with their experimental values.

2. THEORETICAL CONSIDERATIONS

Fission neutrons are emitted with an energy distribution. There are various models which seek to describe the neutron emission process and there are semi-empirical formulas for representing the neutron energy distribution, or rather, the fission spectrum. In this paper two of these distributions are analysed.

2.1. Fission spectra

The Maxwellian and the Watt spectra, used in the past as weighting functions in dosimetry calculations, are based on simplified models. The new representation developed by Madland and Nix is based on the standard theory of nuclear evaporation, taking into consideration the movement of fission fragments, the distribution of the excitation energy of these fragments and the energy dependence of the cross-section for the process of compound nucleus formation. The two latter effects are disregarded by the Maxwellian and Watt spectra.

The Watt fission spectrum is given by the equation

$$\chi(E) = k.\sinh\sqrt{bE}.\ \exp(-E/a), \tag{1}$$

where the parameters a and b vary according to the material and the energy of the fission-inducing neutrons and k is a normalization constant.

In the Madland-Nix model, the fission spectrum is expressed by

$$\chi(E) = \frac{1}{2}\left[\chi(E,\ E_f^L) + \chi(E,\ E_f^H)\right] , \tag{2}$$

where $\chi(E,\ E_f^L)$ and $\chi(E,\ E_f^H)$ represent, respectively, the spectral components due to light and heavy fission fragments, and E_f^L and E_f^H are the average kinetic energies per nucleon of these fragments.

The two components of this spectrum are defined by

$$\chi(E,\ E_f) = \frac{1}{3(E_f.T_m)^{1/2}}\left[\mu_2^{3/2}E_1(\mu_2) - \mu_1^{3/2}\ E_1(\mu_1) + \right.$$

$$\left. +\gamma(\ \frac{3}{2},\mu_2) - \gamma(\frac{3}{2},\ \mu_1)\right] , \tag{3}$$

with

$$E_1(x) = \int_x^{\infty} \frac{\exp(-\mu)d\mu}{\mu} \quad \text{(exponential integral)} \quad ,$$

$$\gamma(z,x) = \int_0^x \mu^{z-1} \exp(-\mu)\, d\mu \quad \text{(incomplete gamma function)} \quad ,$$

$$\mu_1 = (\sqrt{E} - \sqrt{E_f})^2/T_m \quad , \tag{4}$$

$$\mu_2 = (\sqrt{E} + \sqrt{E_f})^2/T_m \quad , \tag{5}$$

$$E_f^L = \frac{A_H}{A_L} \frac{\langle E_f^{tot} \rangle}{A} \quad , \tag{6}$$

$$E_f^H = \frac{A_L}{A_H} \frac{\langle E_f^{tot} \rangle}{A} \quad , \tag{7}$$

where,

A ≡ mass number of the compound nucleus,

A_H ≡ mass number of the heavy fission fragment, and

A_L ≡ mass number of the light fission fragment.

T_m, the maximum temperature of the residual nucleus of the fission fragment, is defined by the average initial excitation energy of the fragment, $\langle E^* \rangle$, as

$$T_m = (\langle E^* \rangle / a')^{1/2} \quad , \tag{8}$$

where,

a' ≡ a level density parameter, used like A/10 MeV, to simulate the energy dependence of the cross-section for formation of the compound nucleus,

$$\langle E^* \rangle = \langle E_r \rangle + B_n + E_n - \langle E_f^{tot} \rangle, \qquad (9)$$

$\langle E_r \rangle$ ≡ average energy released in the fission process,

B_n ≡ neutron separation energy,

E_n ≡ fission neutron energy, and

$\langle E_f^{tot} \rangle$ ≡ total kinetic energy of the average fission fragment.

The constants used in determining the spectra are shown in Tables 1 and 2, which consider the fission of ^{235}U induced by thermal (0.025 eV) neutrons and the spontaneous fission of ^{252}Cf.

In Figs 1-4 we show the representative curves for the Watt and the Madland-Nix theoretical fission spectra for ^{235}U and ^{252}Cf.

In the dosimetry measurements, detector foils of various elements are exposed to a field of neutrons for a specified time. The radioactivity induced in the foil is used as an average cross-section measurement weighted by the neutron spectrum of the experiment.

2.2. Adjustment of spectra

The purpose of adjusting spectra is to obtain a form which represents more satisfactorily the real neutron spectrum, or rather, the experimental spectrum to which the activation detectors were exposed. Spectrum adjustment by the least squares method on the basis of experimental measurements is accomplished by solving a system of equations of the type

$$a_i^o = \sum_{j=1}^{n} \sigma_j^i \, \phi_j \qquad i = 1, \ldots m, \qquad (10)$$

where,

a_i^o ≡ is a measurement of activity for the reaction i,

σ_j^i ≡ multigroup cross-section for the reaction i,

$\emptyset_j$ ≡ flux of the group j.

Taking into consideration the experimental measurement performed in the fission spectrum (χ), equation (10) can be written as

$$<\sigma_e>_i = \sum_{j=1}^{n} \sigma_j^i \chi_j \quad , \tag{11}$$

where,

$<\sigma_e>_i$ ≡ experimental measurement of the average cross-section for the reaction i,

with

$$\chi_j = \frac{\emptyset_j}{\sum_j \emptyset_j} \quad , \tag{12}$$

which satisfies the normalization

$$\sum_{j=1}^{n} \chi_j = 1 \quad . \tag{13}$$

The STAY'SL program calculates the most probable flux which satisfies equation (11) through minimization of chi square (χ^2). A brief description of the calculation procedures of the STAY'SL program and the programs used for adjusting the spectra are found in Annex A.

The minimum value of χ^2(χ^2m) is also an indicator of the quality of the data. The consistency of the data can be tested by taking into consideration the number of degrees of freedom of the problem. A second test can be carried out by observing the terms of which χ^2m is composed. There are i terms affecting the final value of χ^2m and each term is associated with an experimental measurement. A large contribution to the value of χ^2m is an indication that the measurement in question should be investigated.

2.3. Spectrum adjustment procedure and calculation of one-group cross-sections

For adjustment of the spectrum, the STAY'SL program requires six input data files (see Annex A), which were obtained in the manner described below:

(1) Experimental measurements of cross-sections: Obtained from the literature for 20 nuclides, carried out with the fission spectra of ^{235}U [1,5] and ^{252}Cf [1];

(2) Relative covariance matrix of the experimental measurements: the squares of the experimental errors were used as diagonal elements. The components outside the diagonal were assumed to be zero;

(3) Multigroup flux: A program entitled GROUPM was developed to produce the multigroup flux, on the basis of the analytical expressions of Watt and Madland-Nix;

(4) Multigroup cross-sections: Obtained from ENDF/B-V [4] through processing with the NJOY [6] 187-group program (internal structure, LASL-187, embedded in the code) weighted with the Watt spectrum;

(5) Relative covariance matrix for the flux: this was generated by the FCOV [3] program. The diagonal components of this matrix were considered equal to 0.14, which is the mean between the maximum values of the standard deviation for ^{252}Cf, described by Mannhart [7]. The components outside the diagonal were considered zero;

(6) Relative covariance matrix for the cross-sections: this was obtained by means of the XCOV program [3]. The diagonal components were assumed to be as 10^{-6} and the components outside the diagonal as zero. Since the objective is analysis of the spectrum, an effort was made to minimize the errors in the cross-sections through a low value of covariance.

The average cross-sections for one energy group were calculated with the NJOY program. The input spectra were obtained by the GROUPM (theoretical) and STAY'SL (adjusted) programs.

3. RESULTS

The values of the average cross-sections calculated by using the two representations for the fission spectra of ^{235}U and ^{252}Cf, are presented in Tables 3 and 4. These tables also show the values obtained with weighting by the spectra adjusted by means of the STAY'SL program. The effect of the theoretical

and adjusted spectra is compared by means of the quantity Q, defined as the modulus of the value calculated for the average cross-section divided by the experimental value less unity ($Q = |C/E - 1|$).

In Figs 5 to 8 we present the graphs of the adjusted spectra and, in Figs 9 to 12, the graphs of the relationships between the adjusted and the theoretical spectra.

4. CONCLUSIONS

In the calculation of average cross-sections, the Madland-Nix ($\langle Q \rangle = 0.072$) and Watt ($\langle Q \rangle = 0.070$) representations for the thermal neutron fission spectrum of ^{235}U are found to be equivalent. For the spontaneous fission of ^{252}Cf, the Madland-Nix representation proves to be the most suitable.

The calculations performed with the adjusted spectra show the efficiency of the adjustment method. In Tables 3 and 4 we observe considerably lower values of Q for the cases of the adjusted spectra.

Because of its inclusion of effects which were disregarded in earlier representations, the Madland-Nix spectrum will probably be included in new versions of ENDF/B.

This analysis suggests that, in the experimental determination of the fission spectrum, the energy band between 0.5 and 20.0 MeV should be considered in greater detail. The major deviations in respect of the spectrum as well as a shortage of experimental measurements for average cross-sections are found in this range.

By way of a suggestion for future study, the influence of complete covariance matrices in the adjustment of spectra should be investigated.

ANNEX A

A.1. STAY'SL program

To carry out the adjustment of the spectrum, the STAY'SL requires six input files, already specified in section 2.3.

Figure 13 is the block diagram for using the STAY'SL program.

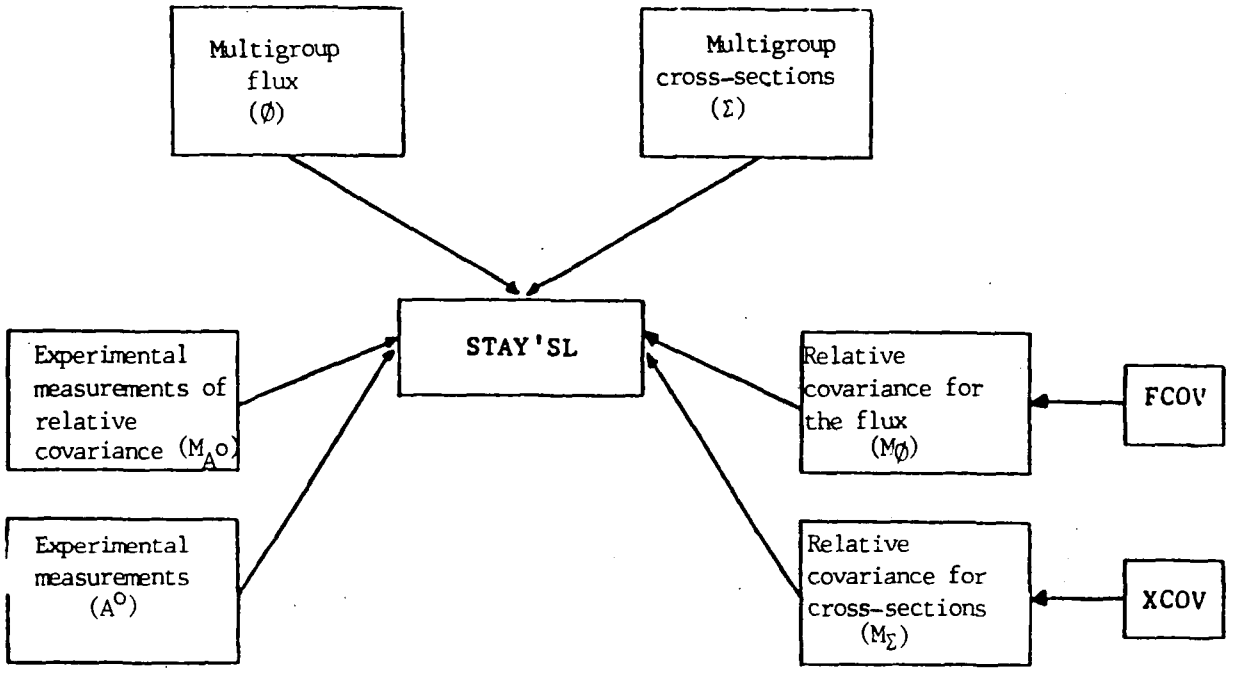

Fig. 13. Input files for the STAY'SL program.

The output flux $\emptyset'_j$, its relative covariance matrix, $M'_\emptyset$, and the minimum value of χ^2, $\chi^2 m$, are obtained by the expressions

$$\emptyset'_j = \emptyset_j \left[1 + \sum_{i,k} U_{ij} W_{ik} (a^o_k - a_k) \right] , \tag{14}$$

$$m_{\emptyset' k\ell} = m_{\emptyset k\ell} - \sum_{i,j} W_{ik} U_{ik} U_{j\ell} \tag{15}$$

and

$$\chi^2_m = \sum_{i,j} (a^o_i - a_i) W_{ij} (a^o_j - a_j) , \tag{16}$$

where

$$W = (N^\Sigma_A + N^\emptyset_A + N_A{}^o)^{-1} , \tag{17}$$

$$N_A{}^o = \tilde{A}^o . M_A{}^o . \tilde{A}^o , \tag{18}$$

$$n^\emptyset_{A\ ij} = \sum_\ell c_{i\ell} \ u_{j\ell} , \tag{19}$$

$$n^\Sigma_{A\ ij} = \sum_{k,L} c_{ik} . m_{\Sigma ij,kL} . c_{jL} , \tag{20}$$

$$U_{ij} = \sum_\ell m_{\emptyset j\ell} . c_{i\ell} \tag{21}$$

$$a_i = \sum_j c_{ij} , \tag{22}$$

$$c_{ij} = \emptyset_j . \sigma^i_j . \tag{23}$$

A.2. Programs for analysis of the neutron spectrum

The programs used for analysing the spectrum can be divided into two classes: the first, comprising programs like SPECTRA, SAND-II and CRYSTAL-BALL [8,9,19], is characterized by the adoption of iterative methods; the second, which includes the DANTE [11] and STAY'SL programs, uses the least-squares method.

The programs using iterative methods take as their starting point an initial spectrum and modify it point by point until the least-squares difference between the measured and the calculated values is within a pre-set limit. These programs require a personal judgement for choosing the solution which is physically acceptable.

The STAY'SL program uses the experimental measurements on initial flux and multigroup cross-sections together with their respective errors. The DANTE program can be classified as a special case of the STAY'SL program inasmuch as the cross-sections are considered as constant. These programs give a solution which is unique and well defined.

The STAY'SL program solves equation (11) for the neutron flux. In order to solve this equation for the flux and the cross section [3,7]; use may be made of the TRY'SL and FERRET programs.

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Table 1. Constants for the Watt spectrum

Fission reaction	a (MeV)	b (1/MeV)	k	Ref.
$^{235}U + n$	0,9880	2,2490	0,43960	4
^{252}Cf	1,0687	2,6912	0,30334	1

Table 2. Constants for the Madland-Nix spectrum [2]

Fission reaction	Light fragment	Heavy fragment	$\langle E_r \rangle$ (MeV)	B_n (MeV)	$\langle E_f^{tot} \rangle$ (MeV)	T_m (MeV)	E_f^L (MeV)	E_f^H (MeV)
$^{235}U + n$	^{96}Sr	^{140}Xe	186,980	6,546	171,800	0,960	1,062	0,499
^{252}Cf	^{108}Mo	^{144}Ba	219,408	0,000	185,900	1,153	0,984	0,553

Table 3. One-group cross-sections for two representations of the thermal fission spectrum of ^{235}U.

Reaction	Experimental value (error) (mb)	Watt	Q	Madland-Nix	Q	Watt (adjusted)	Q	Madland-Nix (adjusted)	Q
Al-27 (n,p)	3,86 (0,25)	4,258	0,103	4,307	0,116	4,108	0,064	4,129	0,070
Al-27 (n,α)	0,705(0,04)	0,7181	0,019	0,7214	0,023	0,7051	0,000	0,7083	0,005
Ti-47 (n,p)	19,0 (1,4)	22,45	0,182	22,91	0,206	21,91	0,153	22,13	0,165
Ti-48 (n,p)	0,3 (0,018)	0,2812	0,063	0,2829	0,057	0,2756	0,081	0,2770	0,077
Mn-55 (n,2n)	0,244 (0,015)	0,2024	0,170	0,2133	0,126	0,2079	0,148	0,2154	0,117
Fe-54 (n,p)	79,7 (4,9)	81,05	0,017	82,65	0,037	78,58	0,014	79,22	0,006
Fe-56 (n,p)	1,035(0,075)	1,035	0,000	1,041	0,006	1,013	0,021	1,017	0,017
Co-59 (n,α)	0,143(0,01)	0,1499	0,048	0,1507	0,054	0,1470	0,028	0,1477	0,033
Ni-58 (n,p)	108,5 (5,4)	105,0	0,032	107,1	0,013	102,0	0,060	102,9	0,052
Ni-60 (n,p)	2,3 (0,4)	2,608	0,134	2,625	0,141	2,537	0,103	2,548	0,108
Cu-63 (n,α)	0,5 (0,056)	0,5581	0,116	0,5617	0,123	0,5419	0,084	0,5442	0,088
Cu-63 (n,γ)	9,3 (1,4)	9,873	0,062	9,712	0,044	9,912	0,066	9,792	0,053
In-115 (n,n')	189,0 (8,0)	179,2	0,052	182,8	0,033	178,0	0,058	180,2	0,047
In-115 (n,γ)	134,5 (6,0)	124,7	0,073	123,3	0,083	125,7	0,065	125,0	0,071
I-127 (n,2n)	1,05 (0,065)	1,213	0,155	1,237	0,178	1,172	0,116	1,179	0,123
Au-197 (n,γ)	83,5 (5,0)	78,29	0,062	76,53	0,083	78,75	0,057	77,40	0,073
Th-232 (n,f)	81,0 (5,4)	75,01	0,074	76,61	0,054	74,38	0,082	75,35	0,070
Np-237 (n,f)	1312,0 (50,0)	1347,0	0,027	1361,0	0,037	1346,0	0,026	1357,0	0,034
U-238 (n,f)	305,0 (10,0)	305,1	0,000	311,7	0,022	303,0	0,007	307,1	0,007
Pu-239 (n,f)	1811,0 (60,0)	1791,0	0,011	1794,0	0,009	1792,0	0,010	1795,0	0,009
			$\langle Q \rangle$=0,070		$\langle Q \rangle$=0,072		$\langle Q \rangle$=0,062		$\langle Q \rangle$=0,061

Table 4. One-group cross-sections for two representations of the spontaneous fission spectrum of ^{252}Cf.

Reaction	Experimental value (error) (mb)	Watt	Q	Madland-Nix	Q	Watt (adjusted)	Q	Madland-Nix (adjusted)	Q
Na-23 (n,γ)	0,335(0,015)	0,2546	0,240	0,2589	0,227	0,2609	0,221	0,2641	0,212
Al-27 (n,p)	5,1 (0,5)	6,655	0,305	6,207	0,217	5,220	0,024	5,187	0,017
Al-27 (n,α)	1,006(0,022)	1,476	0,467	1,381	0,373	1,053	0,047	1,049	0,043
Ti-46 (n,p)	13,8 (0,3)	17,46	0,265	16,27	0,179	13,75	0,004	13,66	0,010
Ti-48 (n,p)	0,42 (0,01)	0,5661	0,348	0,5307	0,264	0,4193	0,002	0,4172	0,007
Mn-55 (n,2n)	0,58 (0,06)	0,6286	0,084	0,6419	0,107	0,5996	0,034	0,6075	0,047
Fe-54 (n,p)	84,6 (2,0)	107,1	0,266	101,7	0,202	89,78	0,061	89,18	0,054
Fe-56 (n,p)	1,45 (0,035)	1,927	0,329	1,793	0,237	1,440	0,007	1,432	0,012
Co-59 (n,α)	0,20 (0,01)	0,2996	0,498	0,2803	0,402	0,2192	0,096	0,2182	0,091
Co-59 (n,2n)	0,57 (0,06)	0,5767	0,012	0,5917	0,038	0,5534	0,029	0,5630	0,012
Ni-58 (n,p)	118,0 (3,0)	137,2	0,163	130,5	0,106	116,0	0,017	115,2	0,024
Cu-63 (n,γ)	10,95 (0,51)	8,98	0,180	9,162	0,163	9,346	0,146	9,440	0,138
In-115 (n,n')	198,0 (5,0)	200,2	0,011	196,1	0,010	188,9	0,046	187,5	0,053
In-115 (n,γ)	125,3 (4,3)	112,3	0,104	114,9	0,083	119,9	0,043	120,5	0,038
Au-197 (n,γ)	79,9 (2,9)	68,47	0,143	70,5	0,118	72,55	0,092	73,61	0,079
Th-232 (n,f)	89,0 (9,0)	88,57	0,005	86,09	0,033	80,86	0,091	80,30	0,098
U-235 (n,f)	1203,0 (30,0)	1236,0	0,027	1237,0	0,028	1236,0	0,027	1236,0	0,027
Np-237 (n,f)	1332,0 (37,0)	1411,0	0,059	1400,0	0,051	1391,0	0,044	1383,0	0,038
U-238 (n,f)	320,0 (9,0)	350,6	0,096	342,3	0,070	326,5	0,020	324,1	0,013
Pu-239 (n,f)	1804,0 (45,0)	1804,0	0,000	1802,0	0,001	1802,0	0,001	1800,0	0,002
			$\langle Q \rangle$=0,180		$\langle Q \rangle$=0,145		$\langle Q \rangle$=0,053		$\langle Q \rangle$=0,051

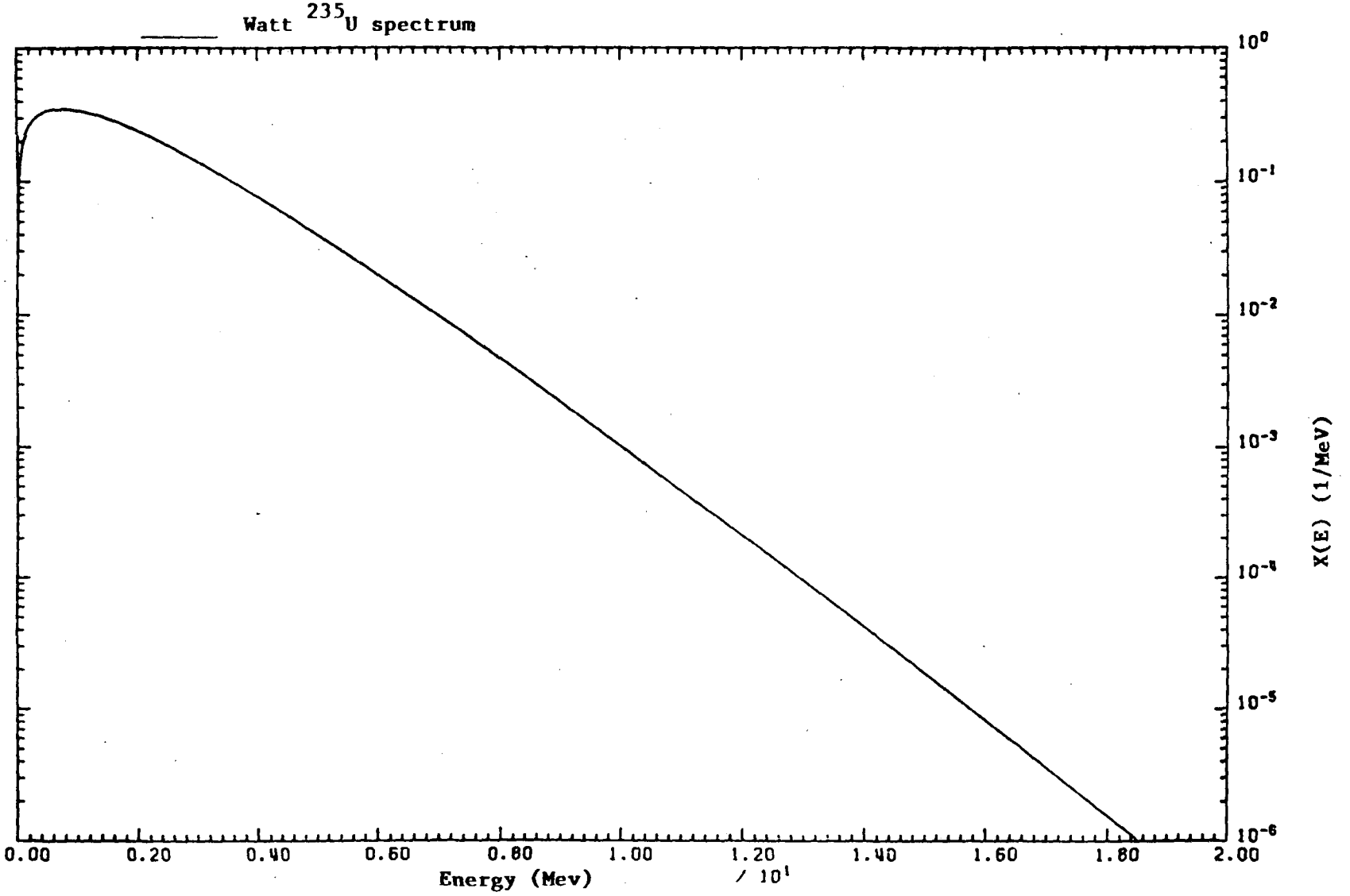

Fig. 1. Watt theoretical fission spectrum – ^{235}U.

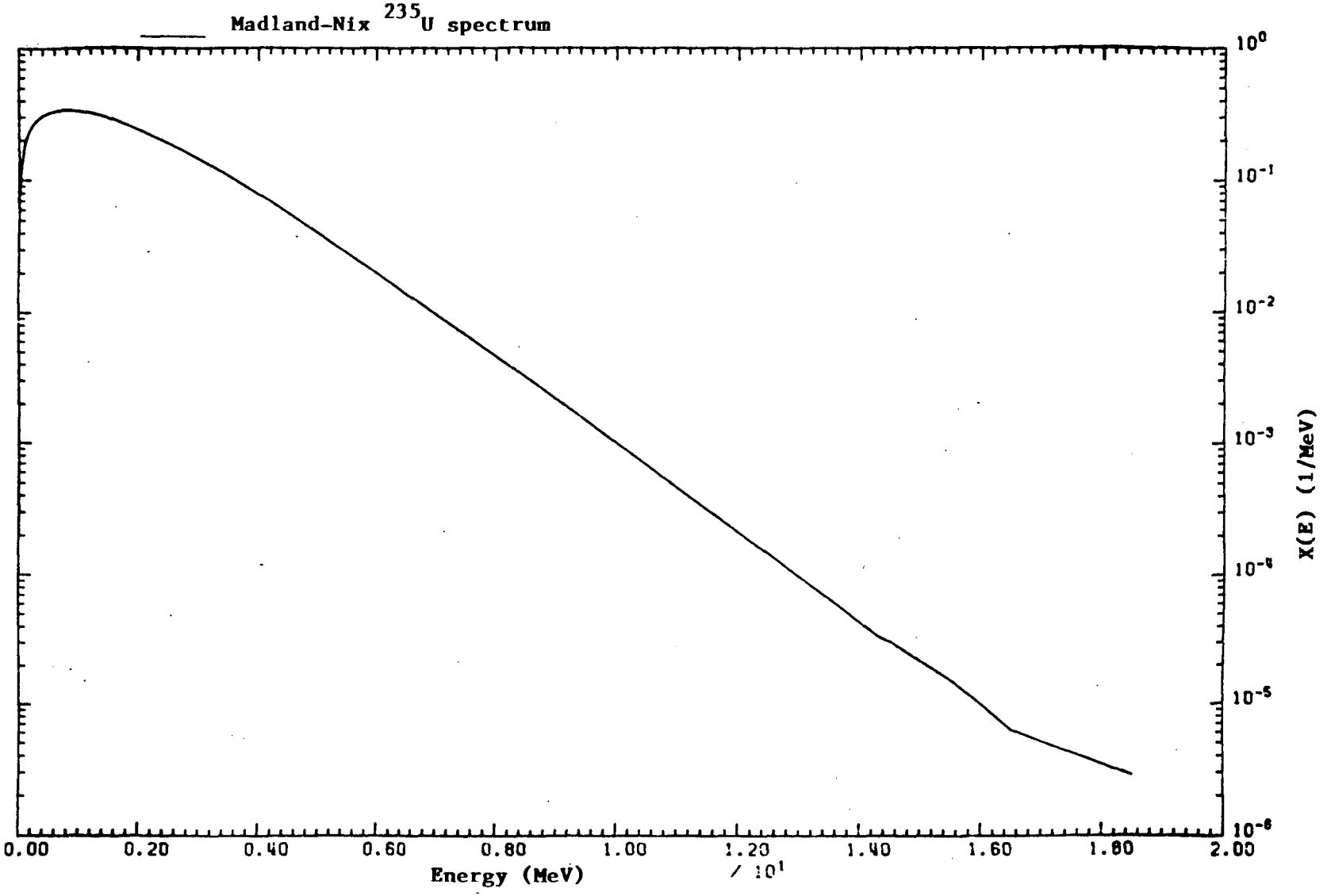

Fig. 2. Madland-Nix theoretical fission spectrum - ^{235}U.

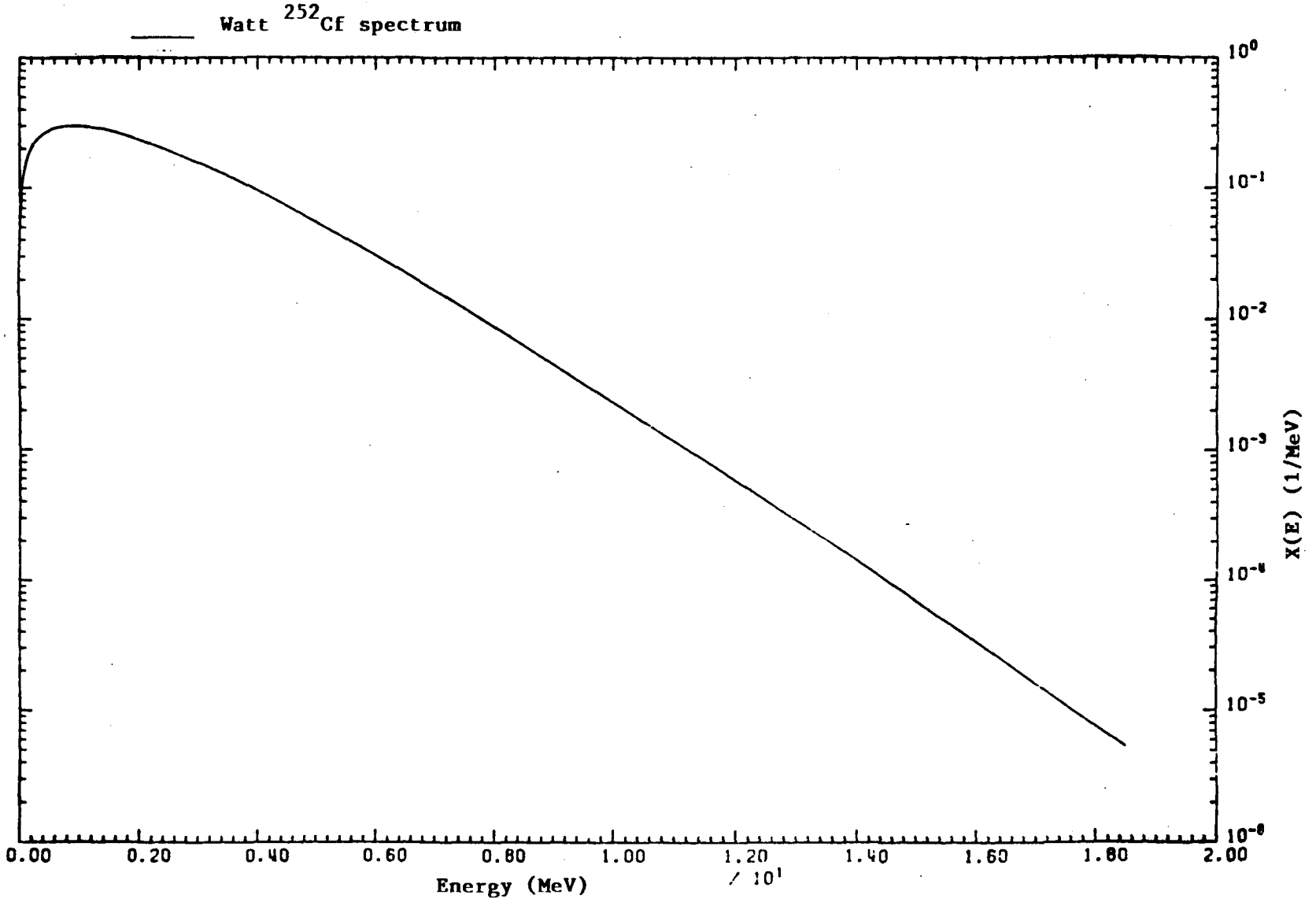

Fig. 3. Watt theoretical fission spectrum - ^{252}Cf.

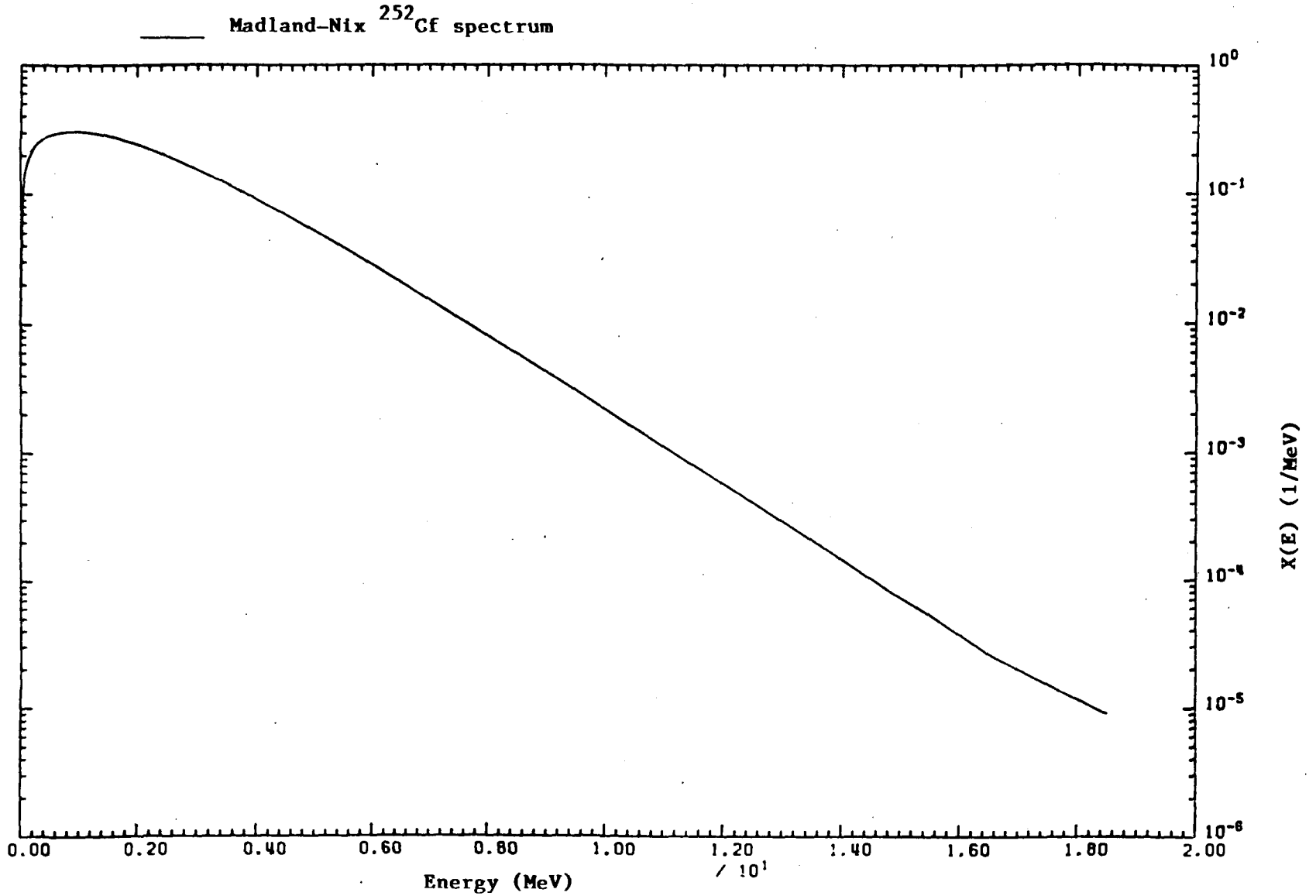

Fig. 4. Madland-Nix theoretical fission spectrum - ^{252}Cf.

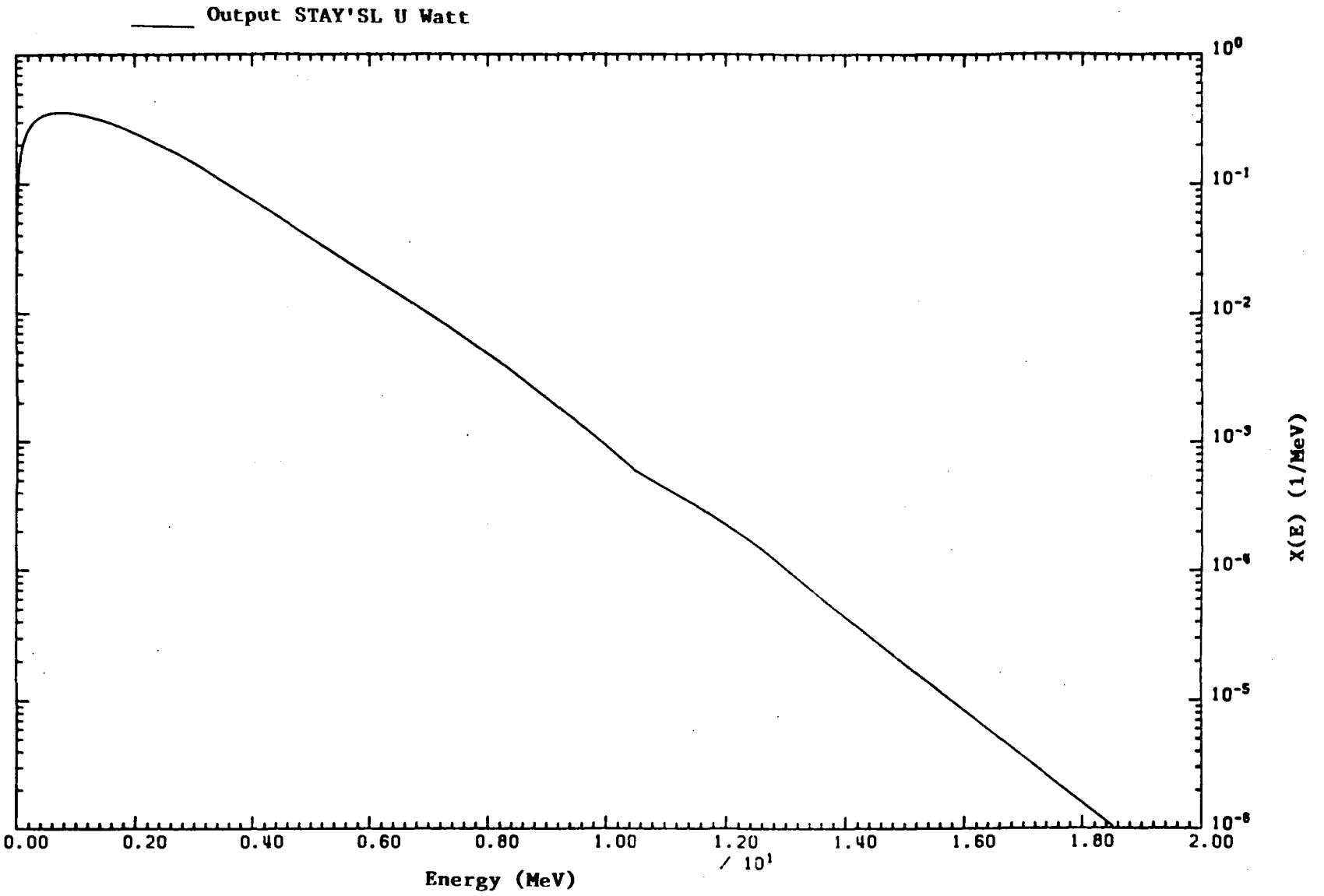

Fig. 5. Adjusted Watt spectrum – ^{235}U.

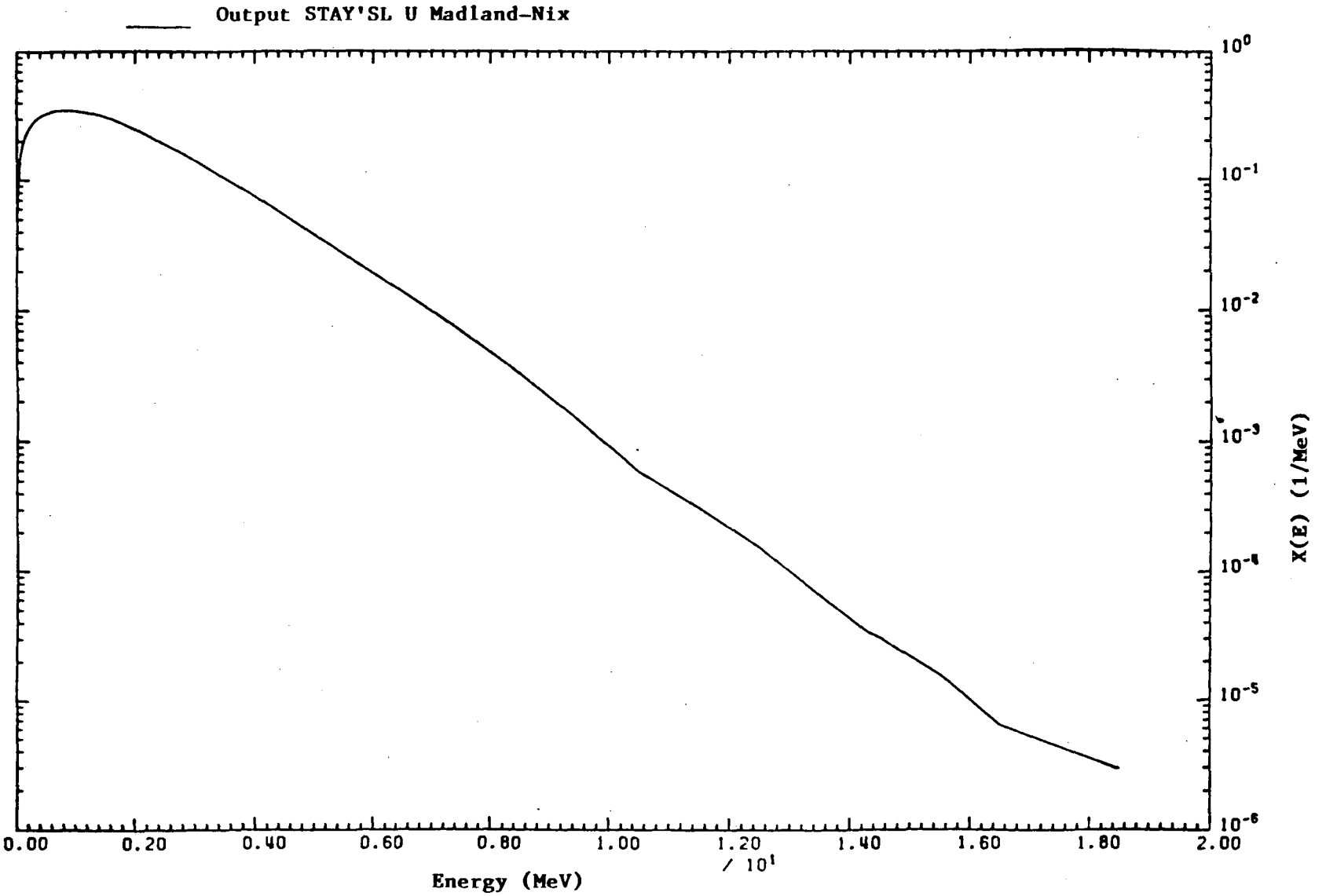

Fig. 6. Adjusted Madland-Nix spectrum – ^{235}U.

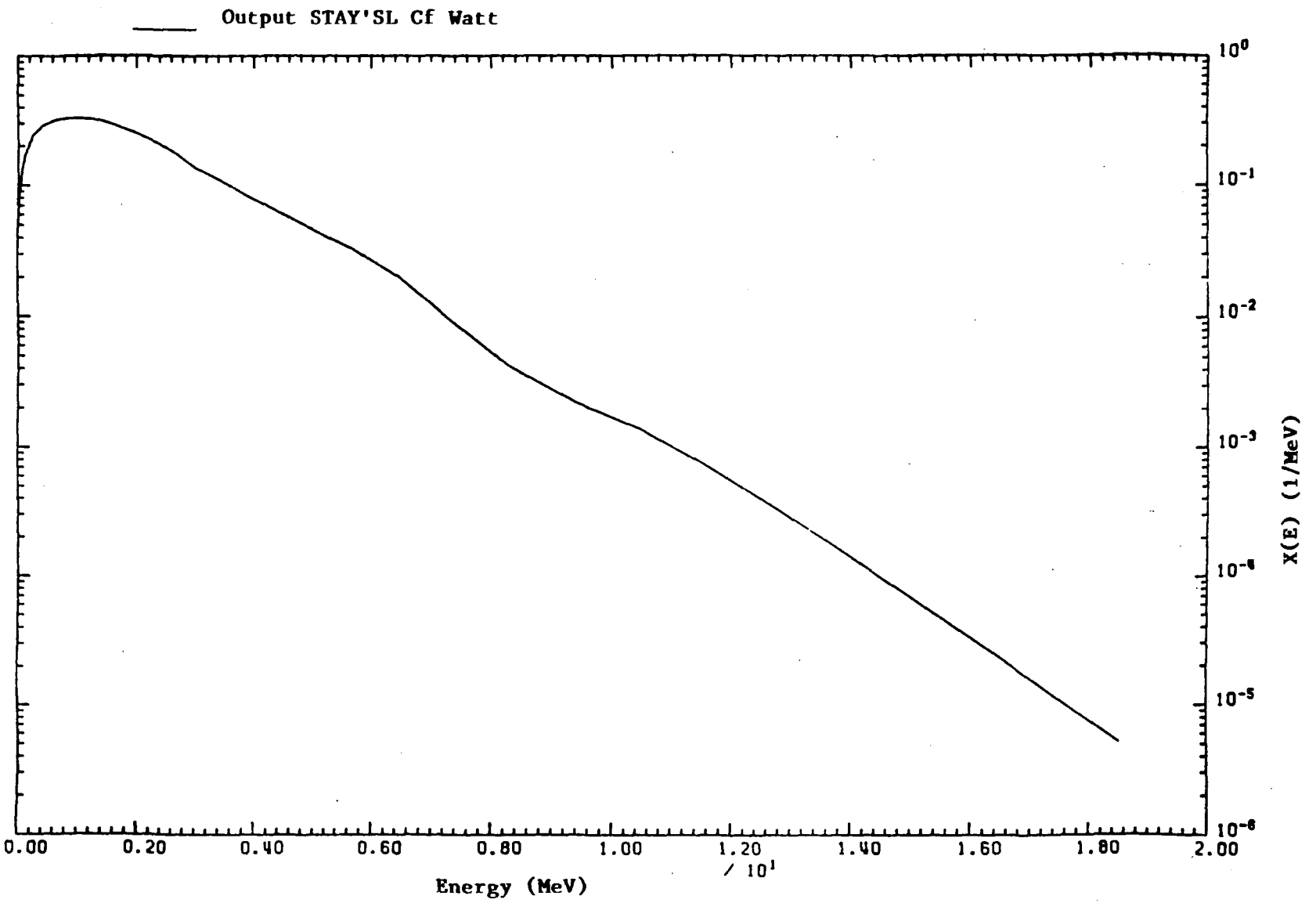

Fig. 7. Adjusted Watt spectrum – ^{252}Cf.

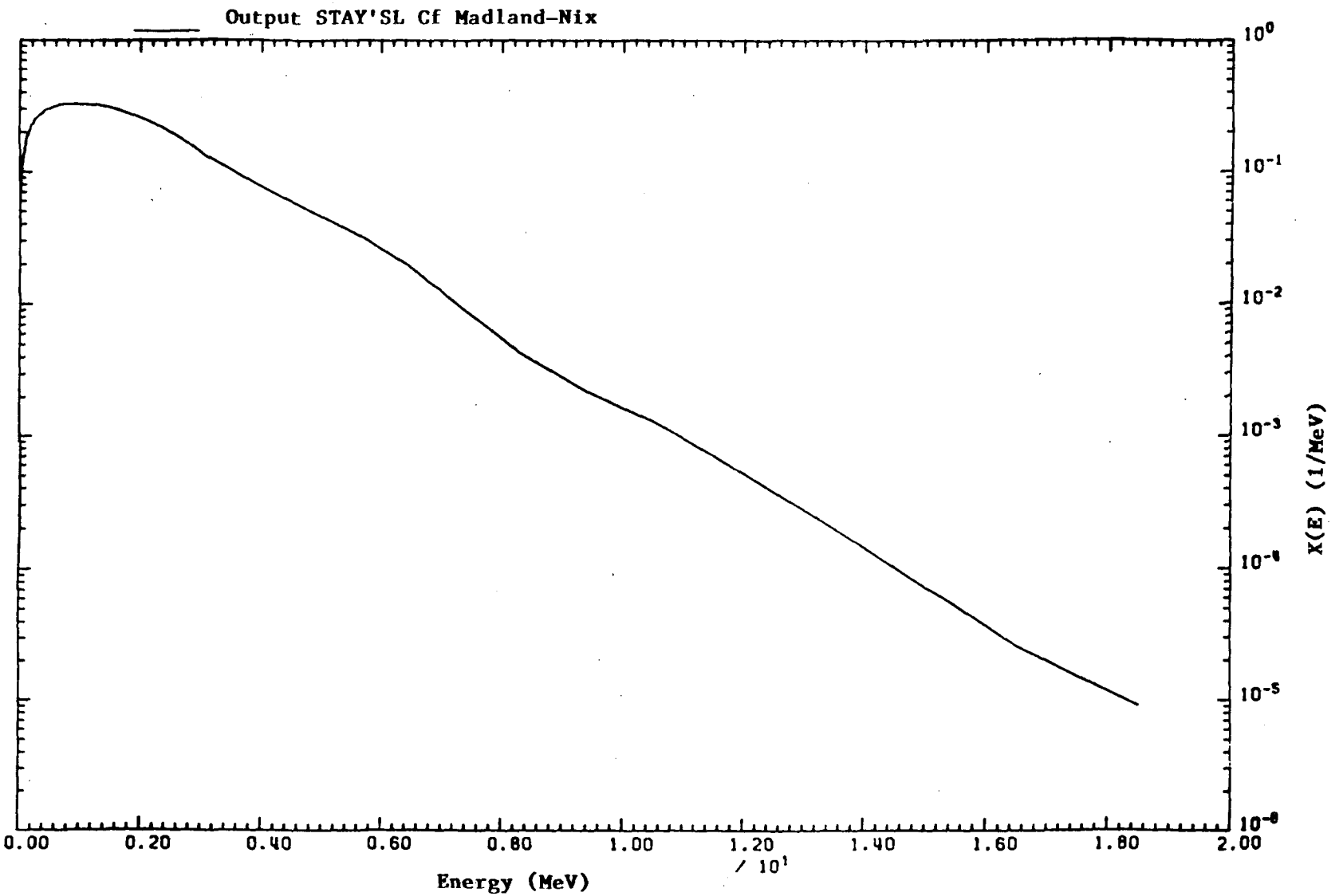

Fig. 8. Adjusted Madland-Nix spectrum - ^{252}Cf.

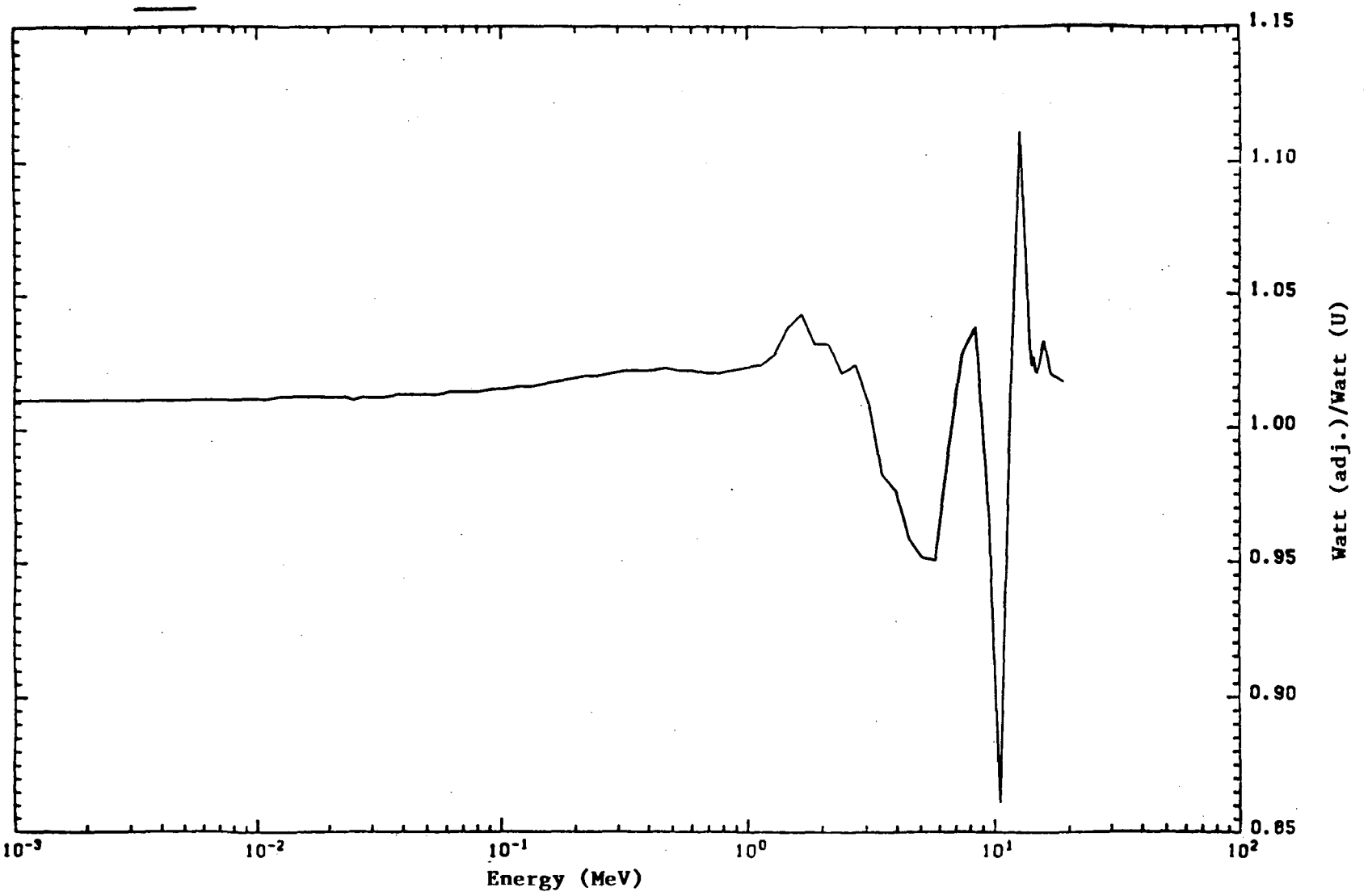

Fig. 9. Relationship between the adjusted and theoretical Watt spectra – ^{235}U.

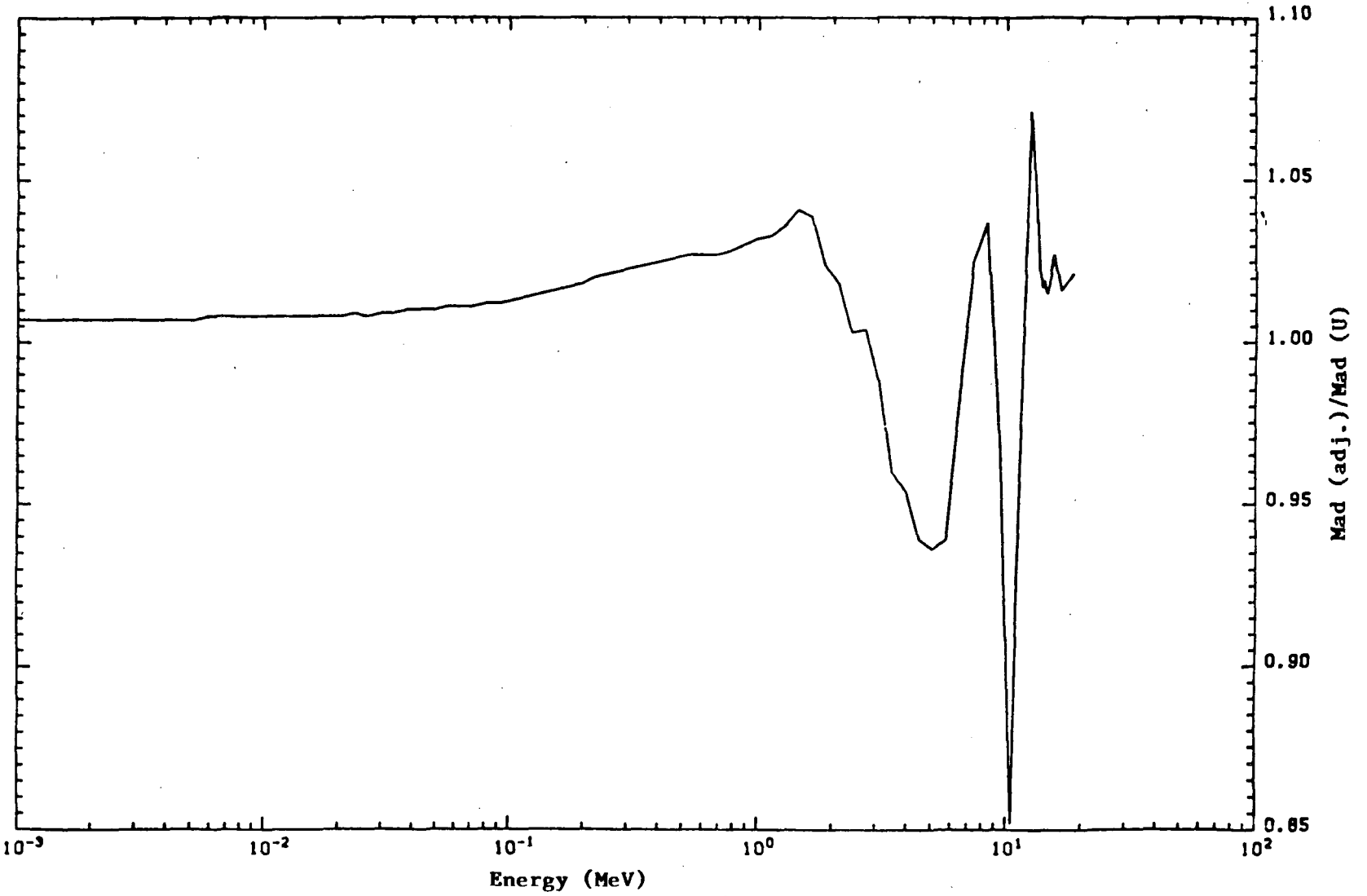

Fig. 10. Relationship between the adjusted and theoretical Madland-Nix spectra - ^{235}U.

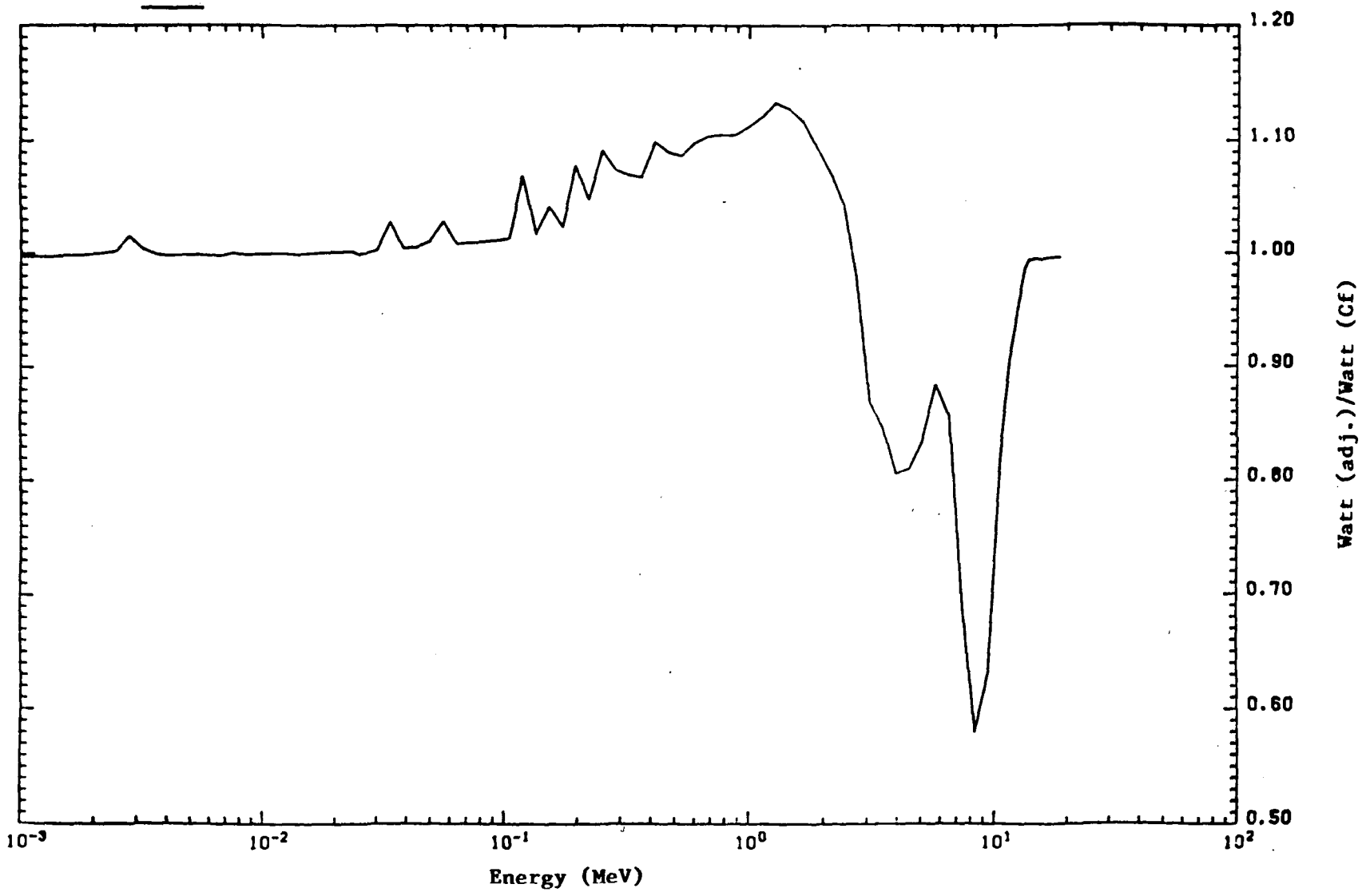

Fig. 11. Relationship between the adjusted and theoretical Watt spectra - ^{252}Cf.

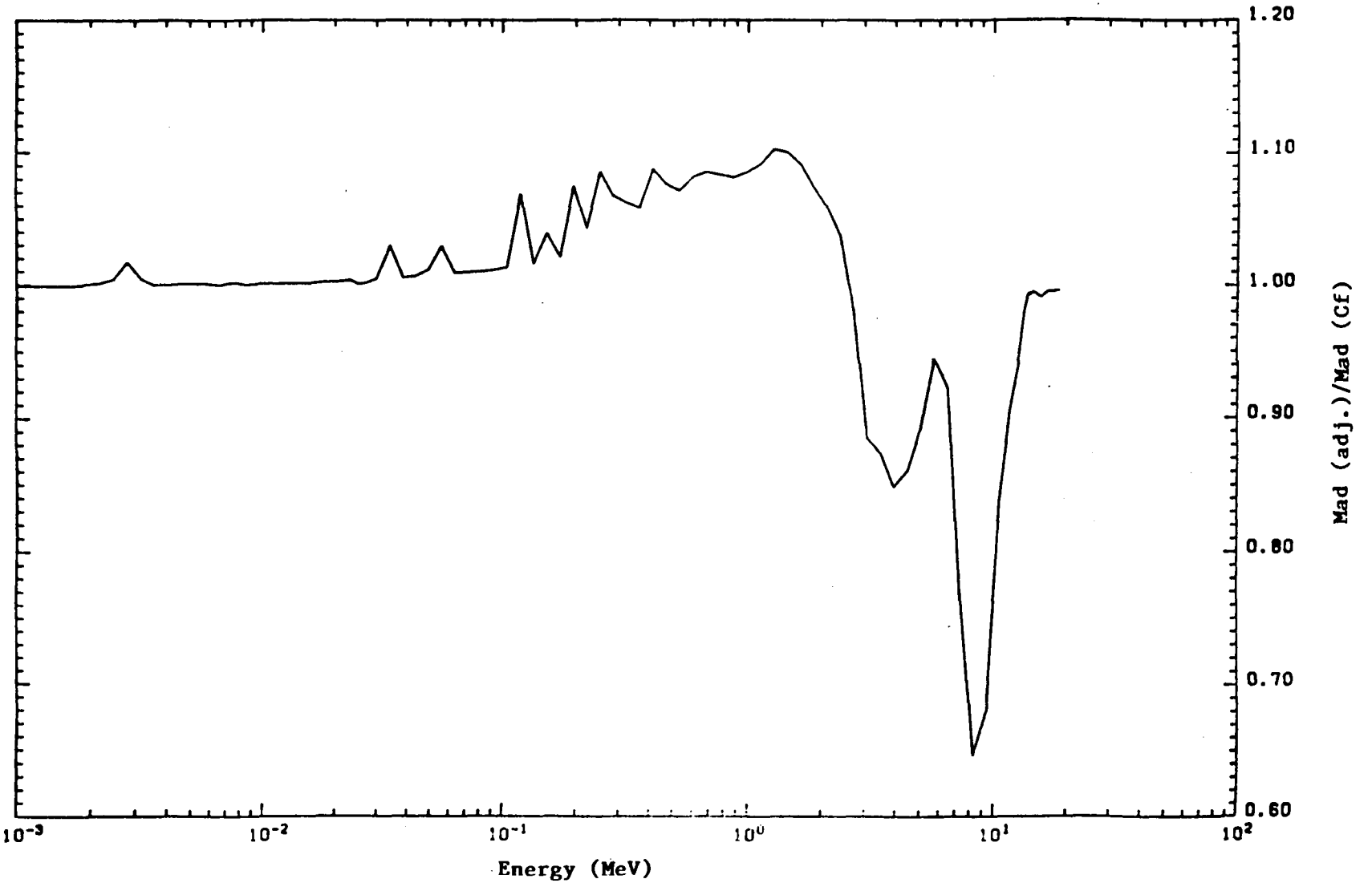

Fig. 12. Relationship between the adjusted and theoretical Madland-Nix spectra – ^{252}Cf.

For Fig. 13 please see page 8