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EVALUATIONS OF THE FE58(n,γ)FE59 AND FE54(n,p)Mn54 REACTIONS FOR THE ENDF/B-V DOSIMETRY FILE

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ABSTRACT

A generalized least-squares adjustment procedure has been used to evaluate two important dosimetry reactions for the ENDF/B-V files. Calculations for the cross section adjustments were made with the computer code FERRET, where input data included both integral and differential experimental data results. For the Fe54 reaction, important ratio measurements were renormalized to ENDF/B-V evaluations of U235(n,f), U238(n,f) and Fe56(n,p). A priori curves which are required for the calculations were obtained using Hauser-Feshbach calculations from the codes NCAP (Fe58) and HAUSER-5 (Fe54). Covariance matrices were also calculated and are included in the evaluations.

Introduction

The Fe58(n,γ)Fe59 and Fe54(n,p)Mn54 reactions have important use as flux-fluence gradient monitors for dosimetry application in fission and fusion reactors. The radioactive reaction products Fe59 and Mn54 are sufficiently long-lived ($t_{1/2}$=45d,1yr) so that they are easily counted. Both of these reactions were previously evaluated by Schenter[1] for the ENDF/B-III and ENDF/B-IV dosimetry files. These evaluations relied on using both integral and differential experimental results.

In this paper we present the results of a re-evaluation of these reactions, where several new aspects of the evaluation process have been incorporated. The most important was use of a generalized least-squares adjustment procedure[2] to obtain an evaluated nominal cross section curve and uncertainty information in the form of a covariance matrix which linked energy points. This procedure involves calculations which use the finite element representation of the FERRET[3] data adjustment code. In addition, recent experimental results were incorporated into the evaluations and ratio data for two important experimental measurements were renormalized to ENDF/B-V data. These new evaluations have been released as part of the ENDF/B-V Dosimetry File.

Fe58(n,γ)Fe59

For ENDF/B-IV the file was mainly based on renormalizing a Hauser Feshbach nuclear models calculation (NCAP computer code)[4] to integral results from the Coupled Fast Reactivity Measurements Facility (CFRMF)[5]. Thermal values were taken from Fabry et al.,[6] and resonance parameters for energies up to 32 KeV were obtained from Hockenbury et al.[7]

Figures 1-3 show the ENDF/B-V evaluation together with the ENDF/B-IV curve and differential experimental data. Input from both differential and integral data and their uncertainties were combined in the FERRET code to produce an "adjusted" continuous capture cross section curve which was used as the basis for the ENDF/B-V result. Also put into the calculation was an "a priori" description which combined multigroup average cross sections obtained from resonance parameters from Garg et al.,[8] for the resolved resonance region (E<300KeV) and ENDF/B-IV for the high energy (E<300KeV) region. The histogram or multigroup cross section description in the resonance region is required for the FERRET least squares calculation because following the exact resonance structure takes too many points for standard computer calculations especially for the covariance matrix part.

Results from six thermal experiments, 30 KeV point by Hong et al.,[9] and resonance parameter determinations up to 300 KeV by Hockenbury et al.,[10] Beer et al.,[11] and Garg et al.,[8] constitute the differential data input. Integral results included CFRMF[5] and resonance integral experimental measurements. As can be seen from the figures, significant differences are shown between the ENDF/B-V and ENDF/B-IV results for the energy range 220 eV to 50 KeV. The ENDF/B-V resonance integral value of 1.27b compared to 1.5 b for ENDF/B-IV is in good agreement with the quoted value of 1.19±.07b given in BNL-325[12].

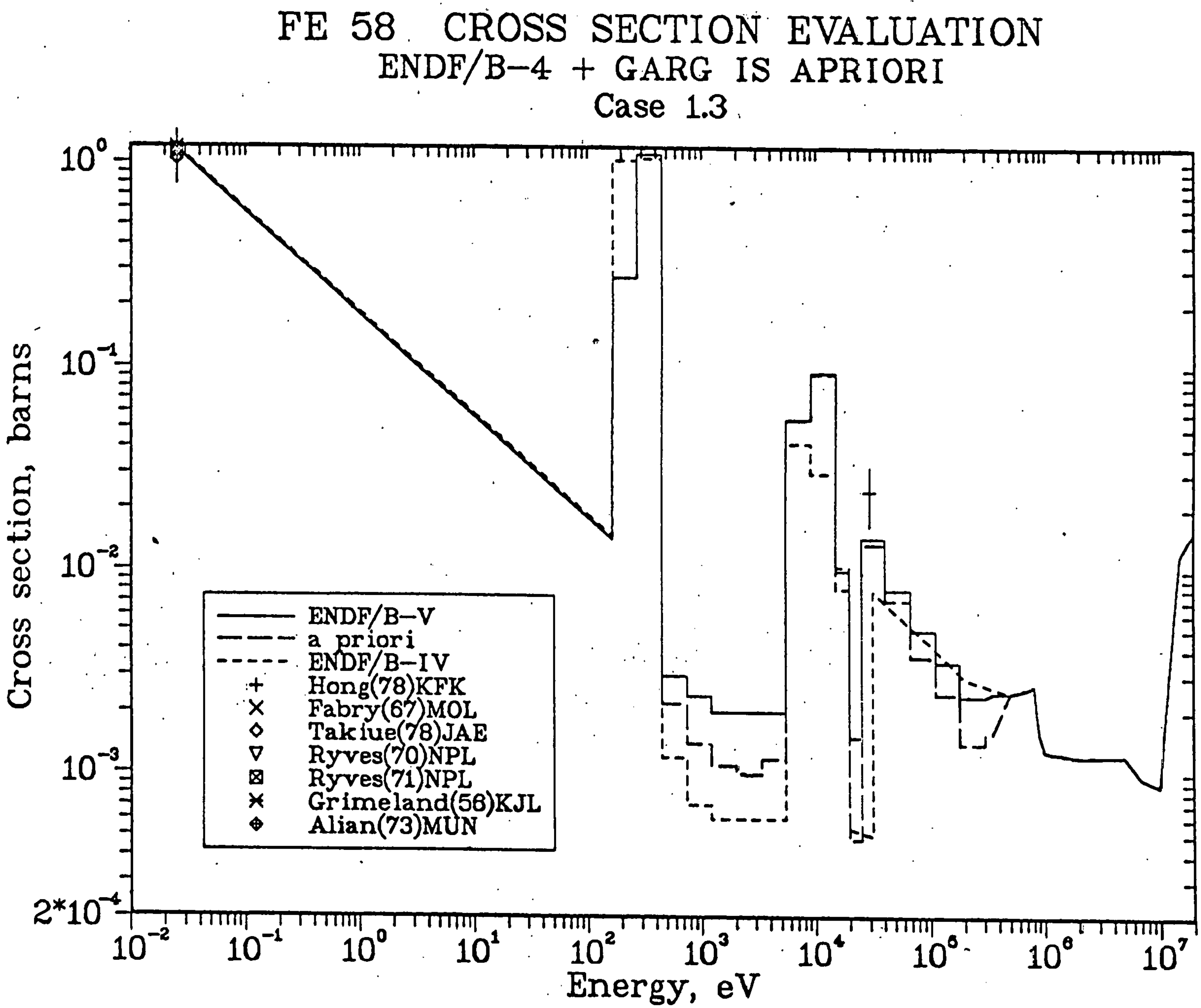

FE 58 CROSS SECTION EVALUATION
ENDF/B-4 + GARG IS APRIORI
Case 1.3
Cross section, barns
Energy, eV
ENDF/B-V
a priori
ENDF/B-IV
Hong(78)KFK
Fabry(67)MOL
Takiue(78)JAE
Ryves(70)NPL
Ryves(71)NPL
Grimeland(56)KJL
Alian(73)MUN

Figure 1.

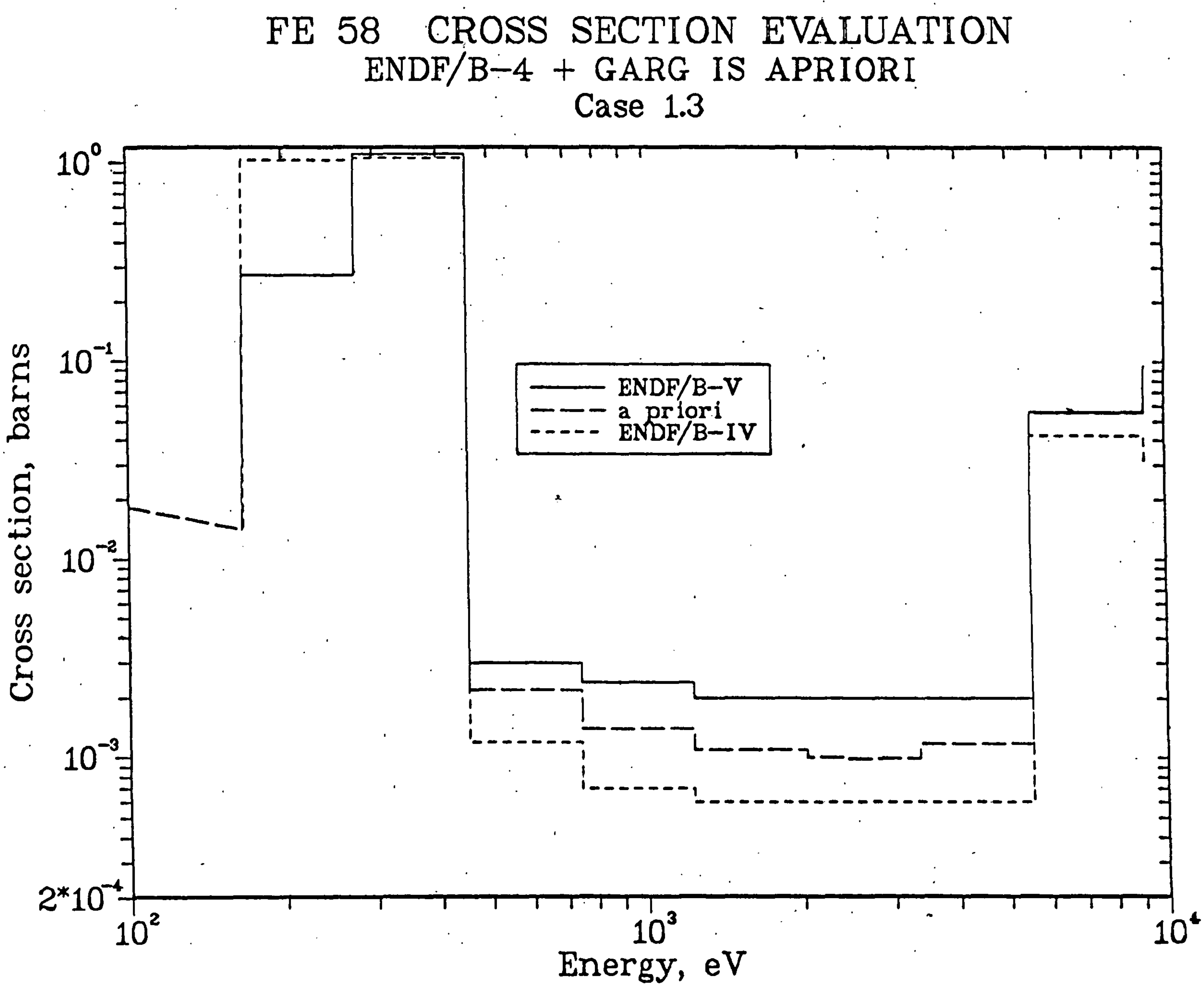

FE 58 CROSS SECTION EVALUATION
ENDF/B-4 + GARG IS APRIORI
Case 1.3
Cross section, barns
Energy, eV
ENDF/B-V
a priori
ENDF/B-IV
10^0
10^{-1}
10^{-2}
10^{-3}
$2*10^{-4}$
10^2
10^3
10^4

Figure 2.

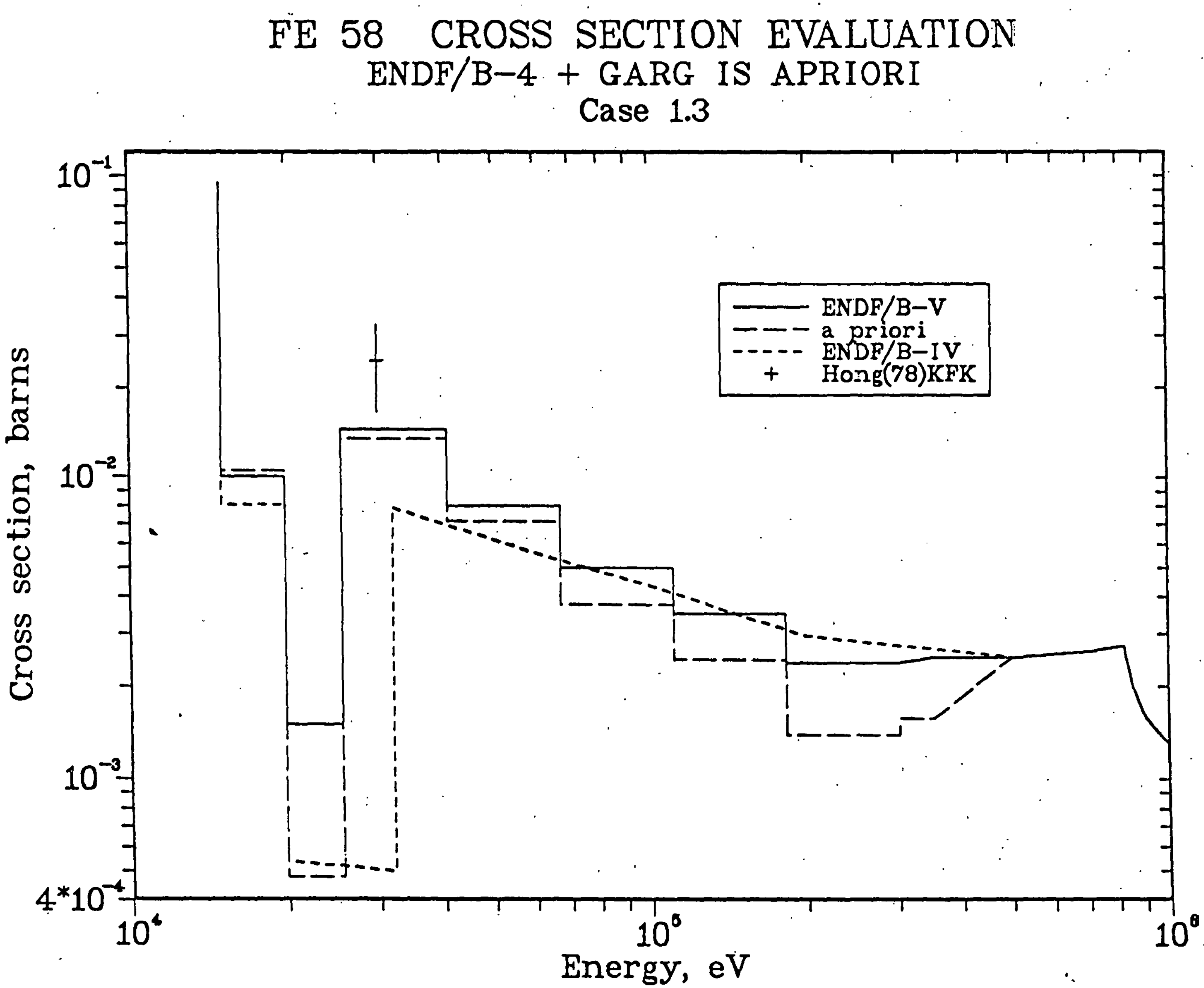

FE 58 CROSS SECTION EVALUATION
ENDF/B-4 + GARG IS APRIORI
Case 1.3
ENDF/B-V
a priori
ENDF/B-IV
Hong(78)KFK
Cross section, barns
Energy, eV
10⁻¹
10⁻²
10⁻³
4*10⁻⁴
10⁴
10⁵
10⁶

Figure 3.

Fe54(n,p)Mn54

Figures 4-8 show the ENDF/B-V and ENDF/B-IV evaluations together with experimental data results and their uncertainties. For ENDF/B-IV the evaluation followed exactly the values of Smith and Meadows[13] below 6.0 MeV and a smooth "eye-guide" curve was contracted which fell between previous evaluations and experimental results above 6.0 MeV.

For ENDF/B-V the direct output from the FERRET code was used. Input to the calculation did not include integral data even though results of measurements exist for CFRMF, EBR-2, U235 and Cf252 fission spectra. All the differential cross section data and uncertainties (statistical and normalization errors) inputted to the calculation are shown in the figures. The two recent experiments indicated by "Smith (75) ANL-V5"[13] and "Paulsen (78) GEEL-V5"[14] were ratio measurements and were renormalized to ENDF/B-V U235 fission (E<4MeV), U238 fission (E>4MeV) for the first and Fe56(n,p) for the second. These renormalizations were substantial, making changes as much as 7% for the Smith and Meadows[13] data and as much as 13% for the Paulsen et al.[14] results.

As previously stated, the FERRET calculation requires a priori nominal curve and covariance matrix. For this Fe54 case a nuclear models calculation using the HAUSER*5[15] code generated the nominal values. It is extremely significant, as can be seen from the figures that the HAUSER*5 calculation predicts the evaluation, since it falls within the experimental data and is surprisingly close to the adjusted curve for almost the entire energy range shown. This is further strengthened since this Hauser Feshbach calculation used no parameters adjusted to previous Fe54 cross section results.

Covariance information for this evaluation is summarized in Table I. The covariance matrix was defined on a set of eight energy intervals that span the range from .1 to 20. MeV. As indicated in Table I, final fractional uncertainties vary from 3.7% near 7 MeV to a maximum of nearly 16% in the lowest energy interval. This 16% is close to the a priori uncertainty and hence reflects the lack of data in this region.

The correlation matrix ρ_{ij} is also tabulated in Table I. Note first that neighboring energy intervals are strongly correlated, a direct consequence of strong short-range correlations that were assumed for the nuclear model calculation. Experimental data extends these correlations somewhat, particularly for the lower energies 2-10 MeV. Finally, note that all correlations are positive. Thus the uncertainties in calculated integral quantities based on this evaluation will be somewhat larger than they would be if the uncertainties in each energy interval were assumed to be statistically independent. If integral data had been included, anticorrelations (negative values for some of the matrix elements ρ_{ij})

would be observed. In that case the uncertainties in integral values could be reduced by a cancellation of uncertainties in contrast to this example.

It can be concluded that progress has been made with this evaluation. The changes from ENDF/B-IV to ENDF/B-V are significant especially between 6 and 12 MeV in addition to adding the covariance information. Integral testing of this data by Magurno[16] shows good agreement with experimental results.

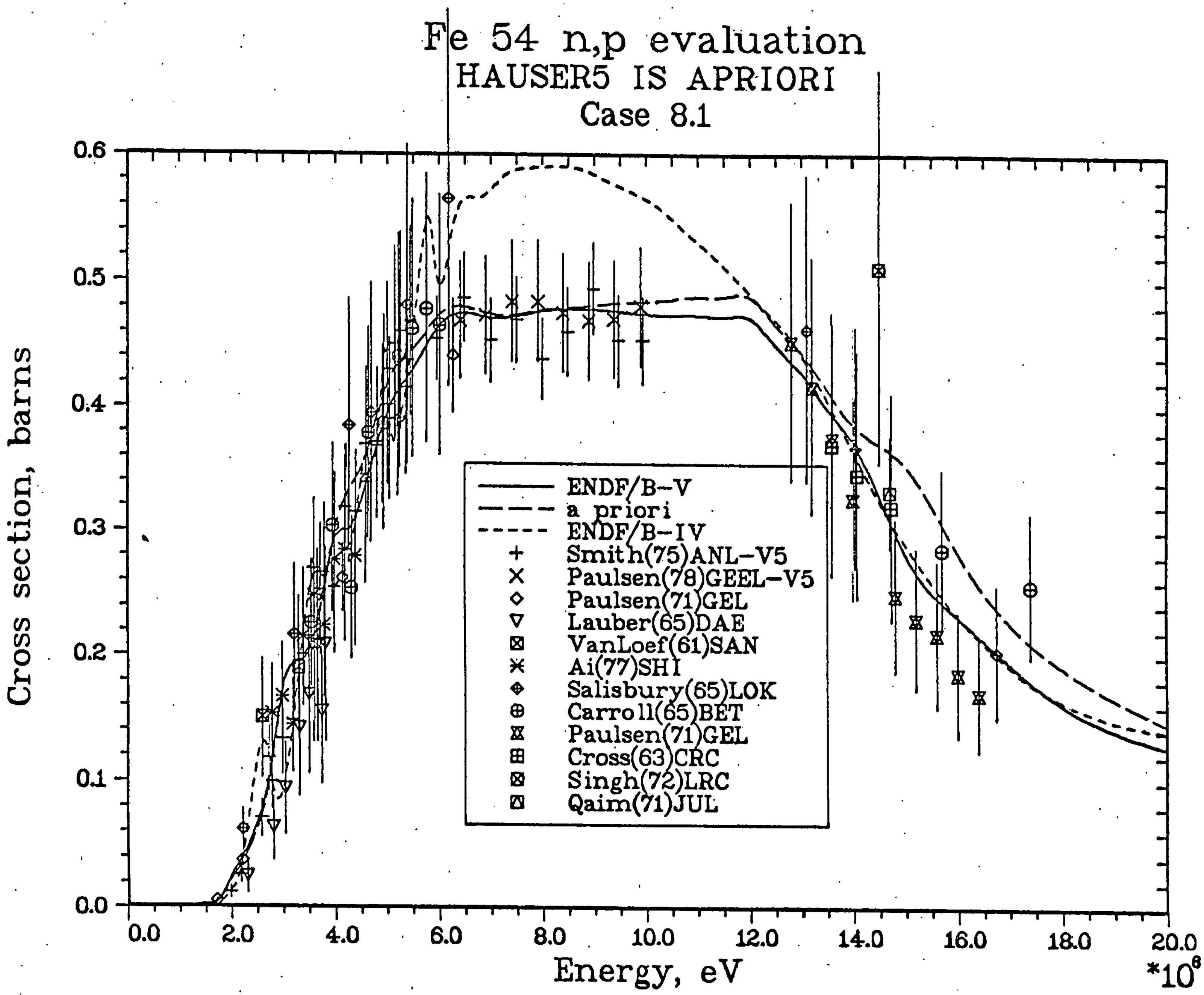
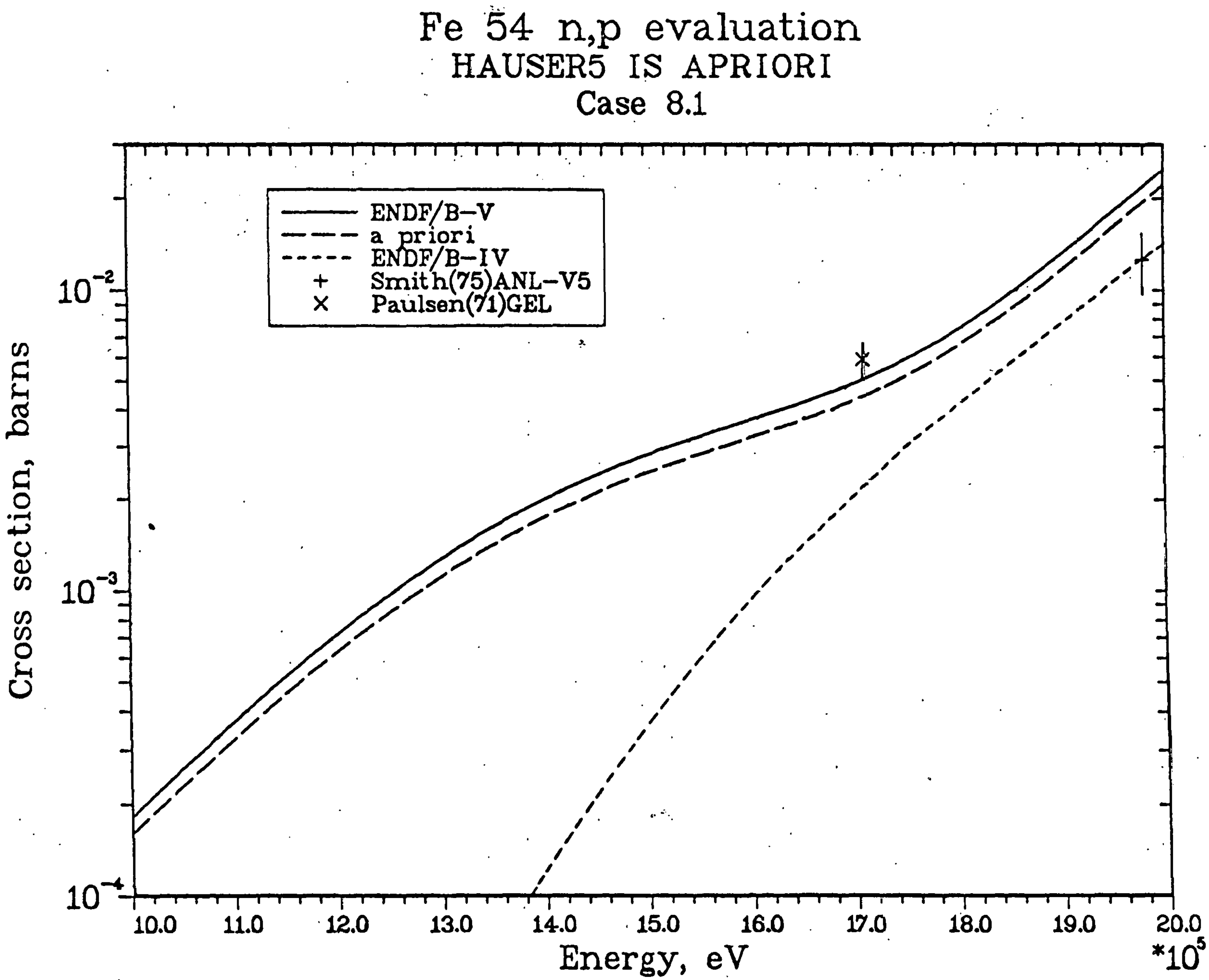

Fe 54 n,p evaluation
HAUSER5 IS APRIORI
Case 8.1
Cross section, barns
Energy, eV
*10^6
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
ENDF/B-V
a priori
ENDF/B-IV
Smith(75)ANL-V5
Paulsen(78)GEEL-V5
Paulsen(71)GEL
Lauber(65)DAE
VanLoef(61)SAN
Ai(77)SHI
Salisbury(65)LOK
Carroll(65)BET
Paulsen(71)GEL
Cross(63)CRC
Singh(72)LRC
Qaim(71)JUL

Figure 4.



Fe 54 n,p evaluation
HAUSER5 IS APRIORI
Case 8.1
ENDF/B-V
a priori
ENDF/B-IV
Smith(75)ANL-V5
Paulsen(71)GEL
Cross section, barns
10^{-2}
10^{-3}
10^{-4}
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
Energy, eV
$*10^{5}$

Figure 5.

Table I. Multigroup uncertainties and correlations obtained for the $^{54}Fe(n,p)$ evaluation.

Energy Intervals (MeV)	0.1	1.0	2.0	4.0	6.0	8.0	12.0	16.0	20.0

Fractional Uncertainty (%)		15.6	7.2	4.7	3.9	3.7	4.4	6.5	9.2
	j \ i	1	2	3	4	5	6	7	8
Correlation Matrix ρ_{ij}	1	1.00							
	2	0.58	1.00						
	3	0.05	0.31	1.00					
	4	0.13	0.29	0.56	1.00				
	5	0.10	0.23	0.38	0.69	1.00			
	6	0.09	0.17	0.28	0.36	0.57	1.00		
	7	0.09	0.13	0.16	0.21	0.14	0.46	1.00	
	8	0.07	0.08	0.10	0.12	0.09	0.12	0.50	1.00

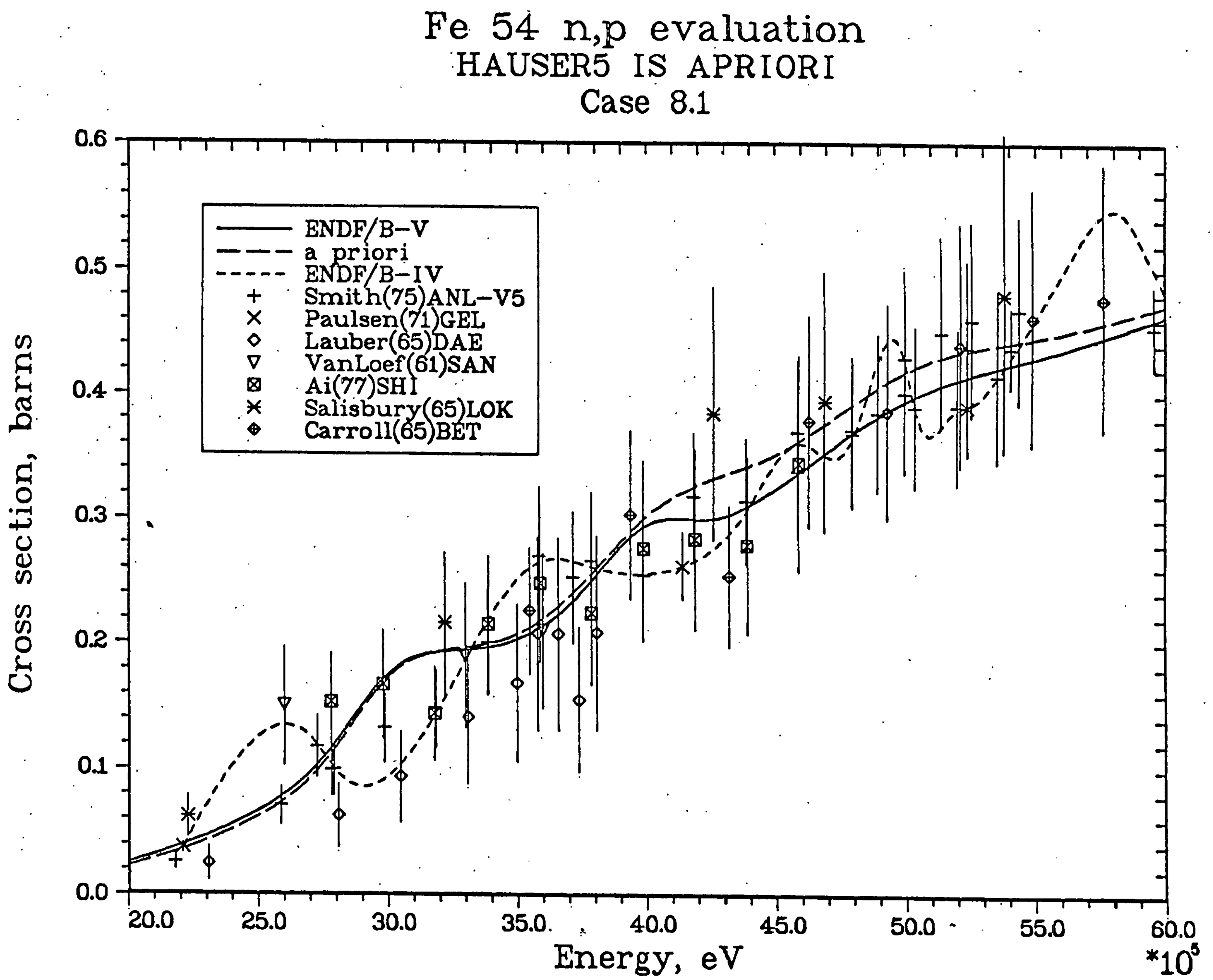

Fe 54 n,p evaluation
HAUSER5 IS APRIORI
Case 8.1
ENDF/B-V
a priori
ENDF/B-IV
Smith(75)ANL-V5
Paulsen(71)GEL
Lauber(65)DAE
VanLoef(61)SAN
Ai(77)SHI
Salisbury(65)LOK
Carroll(65)BET
Cross section, barns
0.0
0.1
0.2
0.3
0.4
0.5
0.6
20.0
25.0
30.0
35.0
40.0
45.0
50.0
55.0
60.0
Energy, eV
*10^5

Figure 6.

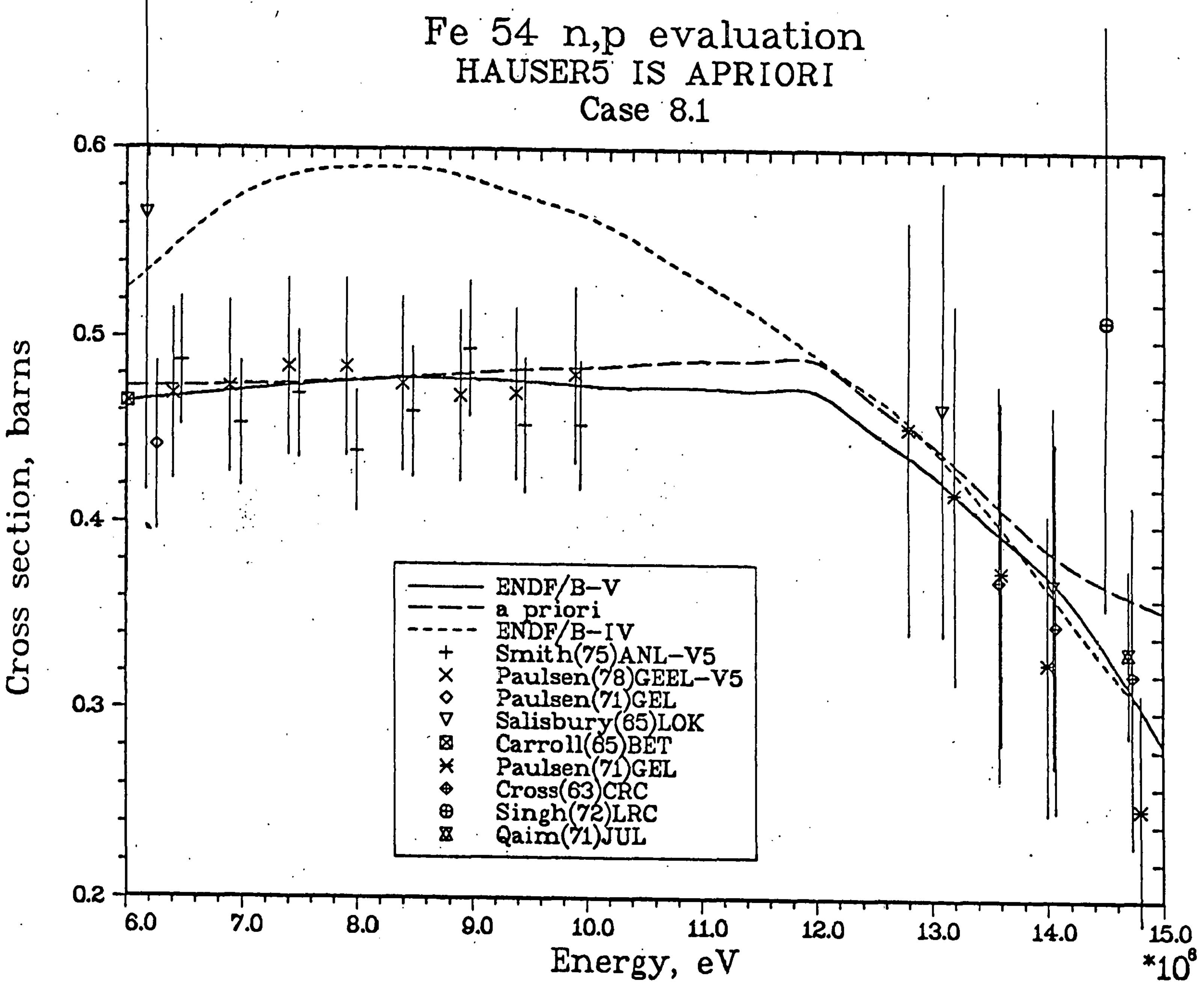
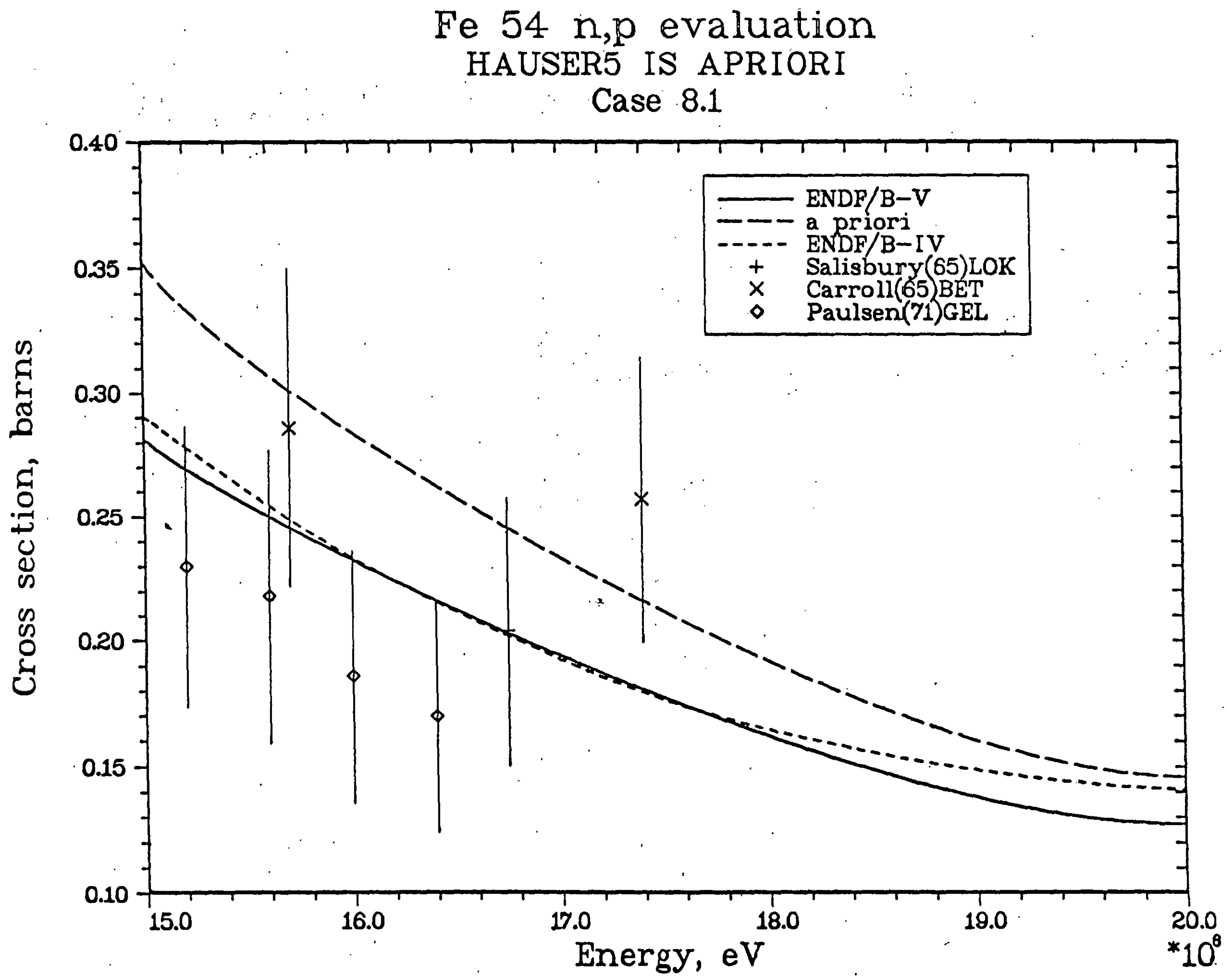

Fe 54 n,p evaluation
HAUSER5 IS APRIORI
Case 8.1
0.6
0.5
0.4
0.3
0.2
Cross section, barns
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
15.0
Energy, eV
*10^6
ENDF/B-V
a priori
ENDF/B-IV
Smith(75)ANL-V5
Paulsen(78)GEEL-V5
Paulsen(71)GEL
Salisbury(65)LOK
Carroll(65)BET
Paulsen(71)GEL
Cross(63)CRC
Singh(72)LRC
Qaim(71)JUL

Figure 7.



Fe 54 n,p evaluation
HAUSER5 IS APRIORI
Case 8.1
ENDF/B-V
a priori
ENDF/B-IV
Salisbury(65)LOK
Carroll(65)BET
Paulsen(71)GEL
Cross section, barns
0.40
0.35
0.30
0.25
0.20
0.15
0.10
15.0
16.0
17.0
18.0
19.0
20.0
Energy, eV
*10^6

Figure 8.

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