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**Comments on Production of Neutron Point Heating
from JEF2 for MCBEND**

by

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1. INTRODUCTION

Local neutron heating data have been generated for core peripheries. The data are in 640 SANDIIa energy groups for use as response functions in the Monte Carlo shielding code MCBEND. Data are available for hydrogen, carbon, oxygen, magnesium, aluminium, silicon, calcium, iron, and zirconium.

This note is a precis of our paper [1] and includes comment on aspects of the data thought to be of interest to the JEF working group. All energies are in eV and resultant heating data are in eV barns.

2. JEF 2.2 EVALUATIONS AND NJOY PROCESSING

Comments on JEF2.2 evaluations for Zr, Fe⁵⁷ and Al²⁷ are included in Appendix 1. This also includes notes on the evaluations for O16 and Si which led to the need to process the files with NJOY91.76.

2.1 Hydrogen

Appendix 2 lists modifications required to NJOY91.76 to process hydrogen data.

We tried to generate all data using both production (NJOY89.62w) and development (NJOY91.76w) versions of NJOY and to set up standard decks for all nuclides. The NJOY91.76w routine BROADR failed while broadening H data from 0 to 293.16K. (This affects very low neutron energies.)

NJOY divides its incident neutron energy grid into panels to process the point data. BROADR has three panels available to searching routines. It searches the middle panel for a required energy. Normally there are many thousand energy points and thus almost always at least 3 panels. However for H there are so few points that not even one panel is filled.

However even that would not matter if Doppler broadening at the highest energy point did not occur. The user can specify the maximum energy for Doppler broadening but we are using 20MeV. NJOY reduces this to the threshold energy of the first inelastic level. In H there is no inelastic so it is left at 20MeV.

The code was searching past the top energy in the panel. In NJOY89.62w it had stopped because variables left in the "empty" part of store fitted the Fortran "IF" tests. In NJOY91.76w different values are left in the empty store and the code fails. By inserting check

prints we were able to make NJOY89.62w fail in a similar manner and thus felt we had to correct the error.

An extra energy, just above the highest energy, was added at the top of the grid with with the same cross section as at the top energy. This means the code is no longer broadening at the last energy.

3. **KINEMATIC LIMITS**

We have made use of HEATR options to calculate kinematic limits. We have included graphs of data which are outside of the limits. Al, Fe⁵⁷ and Zr are included.

4. **RESONANCE SHIELDING**

Resonance shielding is important at high energies. We include Table 5 giving the maximum differences between group cross-sections weighted using the vitamin J spectrum and those weighted with the product of this and $1/\sigma_T$. results for Fe⁵⁶ are graphed.

4.1 **Processing of Unresolved Resonance in Fe⁵⁶**

Due to the interest in resonance shielding we have included Appendix 5 which comments on the JEF 2.2 ENDF/B-VI Fe⁵⁶ data in the unresolved range.

REFERENCE

- [1] C J Dean, C R Eaton
Neutron Cross Sections for Heating in Reactor Shields
AEA-RS 5541 (August 1993)

Appendix 1. Comments on JEF2.2 Evaluations Resulting from Problems with Heating Results

Fe57

The results from processing JEF2 give negative point heating in several groups thus

Group	Energy (eV)		Heating
366	1.2750E+04	1.3500E+04	2.440E+03
367	1.3500E+04	1.4250E+04	3.897E+03
368	1.4250E+04	1.5000E+04	2.002E+03
369	1.5000E+04	1.6000E+04	-8.390E+02
370	1.6000E+04	1.7000E+04	-1.103E+03
371	1.7000E+04	1.8000E+04	-5.192E+02
372	1.8000E+04	1.9000E+04	1.061E+03
373	1.9000E+04	2.0000E+04	1.933E+03
374	2.0000E+04	2.1000E+04	4.142E+03
375	2.1000E+04	2.2000E+04	8.208E+03
376	2.2000E+04	2.3000E+04	1.170E+04
377	2.3000E+04	2.4000E+04	1.811E+04
378	2.4000E+04	2.5500E+04	3.131E+04
379	2.5500E+04	2.7000E+04	6.210E+04
380	2.7000E+04	2.8000E+04	1.109E+05
381	2.8000E+04	3.0000E+04	1.548E+05
382	3.0000E+04	3.2000E+04	6.841E+04
383	3.2000E+04	3.4000E+04	7.578E+03
384	3.4000E+04	3.6000E+04	-7.866E+03
385	3.6000E+04	3.8000E+04	-7.366E+03
386	3.8000E+04	4.0000E+04	1.649E+04
387	4.0000E+04	4.2500E+04	1.037E+05
388	4.2500E+04	4.5000E+04	1.919E+04
389	4.5000E+04	4.7500E+04	5.470E+03
390	4.7500E+04	5.0000E+04	-5.195E+03
391	5.0000E+04	5.2500E+04	-1.761E+04
392	5.2500E+04	5.5000E+04	-1.203E+04
393	5.5000E+04	5.7500E+04	8.028E+02
394	5.7500E+04	6.0000E+04	2.770E+04
395	6.0000E+04	6.3000E+04	8.072E+04
396	6.3000E+04	6.6000E+04	1.910E+04
397	6.6000E+04	6.9000E+04	1.225E+04
398	6.9000E+04	7.2000E+04	-1.158E+04
399	7.2000E+04	7.6000E+04	-1.114E+04
400	7.6000E+04	8.0000E+04	5.228E+04
401	8.0000E+04	8.4000E+04	-6.036E+03
402	8.4000E+04	8.8000E+04	-1.828E+04
403	8.8000E+04	9.2000E+04	-2.219E+04
404	9.2000E+04	9.6000E+04	-7.642E+03
405	9.6000E+04	1.0000E+05	-2.413E+04
406	1.0000E+05	1.0500E+05	-2.649E+04
407	1.0500E+05	1.1000E+05	-5.371E+02
408	1.1000E+05	1.1500E+05	2.114E+04
409	1.1500E+05	1.2000E+05	-1.943E+04
410	1.2000E+05	1.2750E+05	1.536E+04
411	1.2750E+05	1.3500E+05	4.098E+04
412	1.3500E+05	1.4250E+05	2.696E+04
413	1.4250E+05	1.5000E+05	7.473E+03
414	1.5000E+05	1.6000E+05	-1.112E+04
415	1.6000E+05	1.7000E+05	-5.467E+03
416	1.7000E+05	1.8000E+05	2.966E+03

417	1.8000E+05	1.9000E+05	1.860E+03
418	1.9000E+05	2.0000E+05	2.061E+04
419	2.0000E+05	2.1000E+05	8.775E+03
420	2.1000E+05	2.2000E+05	8.658E+03

Problems are occurring between the threshold of the first inelastic level (1.465500+4 eV) and the top of the resolved resonance range (2.0E5 eV). S wave resonance parameters are not given for Fe57 because:-

```

RESOLVED RESONANCE REGION (UP TO 200 KEV):                2634 1451 21
=====                                                    2634 1451 22
FORMALISM:2-CHANNEL REICH-MOORE (REDUCED R-MATRIX) FOR S-WAVE 2634 1451 23
      (1 ELASTIC, ABOVE 14.4 KEV 1 INELASTIC CHANNEL),      2634 1451 24
      SLW FOR HIGHER-ORDER PARTIAL WAVES.                   2634 1451 25
SINCE 2-CHANNEL REICH-MOORE IS NOT ALLOWED IN ENDF-6 FOR NONFISS2634 1451 26
NUCLEI(AND GENERALISED R-MATRIX FORMAT IS TOO AWKWARD) S-WAVE CR2634 1451 27
SECTIONS WERE GENERATED WITH KFK-PROGRAM STRUMA /2/ AND STORED 2634 1451 28
IN FILE 3, WITH STATISTICAL TREATMENT OF DISTANT LEVELS. PARAM. 2634 1451 29
FOR ALL HIGHER-ORDER PARTIAL WAVES ARE GIVEN AS P-WAVE RES. PARAM2634 1451 30
IN FILE 2. THE RESONANCE PARAMETER EVALUATION IS BASED MAINLY ON 2634 1451 31
THE FOLLOWING SOURCES (AND EARLIER WORK REFERENCED THERE)    2634 1451 32
  0 - 200 KEV  BARN BOOK          MUGHABGHAB+ 81      /1/, 2634 1451 33
  0 - 200 "    RESONANCE ANALYSIS PEREY+PEREY 80      /2/, 2634 1451 34
  0 - 200 "    KEDAK-4 (= JEF-1)  FROEHNER   77,81   /3/, 2634 1451 35
  0 - 200 "    CAPTURE ANALYSIS   GAYTHER    79      /4/, 2634 1451 36
  0 - 200 "    CAPTURE ANALYSIS   ALLEN+      82      /5/, 2634 1451 37
  0 - 200 "    CAPTURE ANALYSIS   ROHR+       82      /6/, 2634 1451 38
NOTE:/1/, /2/ DISREGARD INELASTIC WIDTHS. HERE THEY ARE TAKEN 2634 1451 39
FROM 2-CHANNEL TRANSMISSION ANALYSIS OF ROHR AND MUELLER 69 /7 2634 1451 40
THE S WAVE.INELASTIC SCATTERING VIA P- AND D-WAVE LEVELS WAS NE-2634 1451 41
GLECTED BECAUSE OF THE SMALL CENTRIFUGAL-BARRIER PENETRABILITIES2634 1451 42
FOR THE SAME REASON SCATTERING TO THE 136.5 KEV (5/2-) LEVEL 2634 1451 43
WAS NEGLECTED (BELOW 200 KEV).                               2634 1451 44

```

The file 3 data thus contain most of the cross section structure. The problem is in inelastic as can be seen from the following edited HEATR output near the inelastic threshold:-

Incident Neutron energy	Elastic	Heating		Capture	
		Inelastic		Total	gamma
		Total	gamma		
9.0640E+03	3.4358E+03	-	-	5.6508E+04	-5.6504E+04
1.8130E+04	1.5761E+03	9.9321E+03	-1.1455E+04	9.2365E+04	-9.2357E+04
3.6267E+04	9.6866E+03	2.6519E+03	-2.2157E+04	3.7382E+04	-3.7378E+04
7.2538E+04	1.6185E+04	6.8960E+02	-3.4049E+04	2.0272E+04	-2.0268E+04

The inelastic gamma contribution is larger than the total inelastic; capture point heating is small but consistent because the evaluation contains multiplicities of gammas.

The first inelastic level contains resonance structure but the total gamma production cross section for inelastic does not. Hence very odd multiplicities of gammas will be obtained by NIPPER(27). However the negative total point heating will be consistent BUT if data sets are mixed very odd results could be obtained.

The negative data in Fe57 were not seen when included in natural Fe.

AL

There is a warning that Al27 has photon emission data for inelastic divided into data for total inelastic (MF=4) and data for (n,n',p) (MF=28). Page 75 of the HEATR write up (23). There is no corresponding (n,n',p) cross section given. HEATR results flag the consistency check.

Also there is a warning in the heading of the file:-

```
MT=51-63 INELASTIC CROSS SECTION TO DISCRETE STATES          1325 1451 118
MT=51 Q=-0.843 MEV MT=56 Q=-3.001 MEV MT=60 Q=-4.409 MEV    1325 1451 119
  52 -1.013          57 -3.678          61 -4.508          1325 1451 120
  53 -2.210          58 -3.956          62 -4.580          1325 1451 121
  54 -2.732          59 -4.055          63 -4.811          1325 1451 122
  55 -2.980                                1325 1451 123
THRES. TO 5 MEV, BASED ON THE (N,NPRIME) DATA OF TO62, WI63, 1325 1451 124
TS61, AND THE (N,NG) DATA OF CH68, MA65, DI71, OR71, DI73. 1325 1451 125
5 TO 9 MEV, BASED ON AN EVALUATION OF SEVERAL MEASUREMENTS 1325 1451 126
GIVEN IN DI71 (TABLE B1).                                1325 1451 127
9 TO 20 MEV, SMOOTH EXTRAPOLATION PASSING THROUGH 14 MEV DATA 1325 1451 128
OF ST65, BO65A.                                         1325 1451 129
MT=64-90 INELASTIC CROSS SECTION TO GROUPS OF DISCRETE STATES 1325 1451 130
IN BANDS CENTERED ABOUT THE Q-VALUES GIVEN BELOW,      1325 1451 131
MT=64 Q=- 5.25 MEV MT=73 Q=- 9.75 MEV MT=82 Q=-14.25 MEV 1325 1451 132
  65 - 5.75          74 -10.25          83 -14.75          1325 1451 133
  66 - 6.25          75 -10.75          84 -15.25          1325 1451 134
  67 - 6.75          76 -11.25          85 -15.75          1325 1451 135
  68 - 7.25          77 -11.75          86 -16.25          1325 1451 136
  69 - 7.75          78 -12.25          87 -16.75          1325 1451 137
  70 - 8.25          79 -12.75          88 -17.375         1325 1451 138
  71 - 8.75          80 -13.25          89 -18.125         1325 1451 139
  72 - 9.25          81 -13.75          90 -18.875         1325 1451 140
THRES. TO 20 MEV, INTEGRATED CROSS SECTION OVER BANDS 1325 1451 141
OBTAINED BY SUBTRACTING MT=51-63 FROM MT=4. CROSS SECTION 1325 1451 142
DIVIDED AMONG BANDS ACCORDING TO A NUCLEAR TEMPERATURE 1325 1451 143
CALCULATION USING TEMP. BASED ON (N,NPRIME) DATA OF TH63, 1325 1451 144
GR53. THE CROSS SECTION TO THE BANDS WITH MT=64-71 WAS 1325 1451 145
ADJUSTED EXTENSIVELY TO PRODUCE AGREEMENT WITH THE 14-MEV 1325 1451 146
MEASUREMENTS OF SECONDARY NEUTRON SPECTRA BY KA72.      1325 1451 147
****PLEASE NOTE THAT MUCH OF THE CROSS SECTION TO BANDS ABOVE EX=1325 1451 148
****9 MEV SUBSEQUENTLY RESULTS IN CHARGED PARTICLE EMISSION. 1325 1451 149
****SINCE THESE DATA ARE NOT INCLUDED EXPLICITLY AS (N,NX) REAC-1325 1451 150
****TIONS, IT IS IMPORTANT THAT USERS INVOLVED IN CERTAIN CALCU-1325 1451 151
****LATIONS (E.G., LOCAL HEATING) BE AWARE OF THIS INFORMATION.1325 1451 152
```

This seems to indicate:-

- a) Level representation is far from exact but may be different and better than that assumed in the gamma production cross section.

- b) Levels $mt=75,78,80,81,83,84,85,86,87,88,90$ lead to decay by proton emission. Examining the first level ($MT=75$) the neutron needs $8.271000+10.75000$ MeV for breakup. The extra decay energy is unimportant in practical reactors because the flux above 18MeV is a very small component.

Examination of the HEATR module of NJOY indicates it may not be exact in processing the reactions where the residual nucleus breaks up. (LR flag not zero or 31) If we consider an n,n' reaction with $LR=28$ the energy remaining after the gamma ray(s) is/are emitted is split between neutron, residual and proton. NJOY HEATR probably splits it between neutron and initial residual. ie it treats it as n,n' rather than $n,n'p$. However this may be correct if there is a two phase reaction ie (n,n',γ) followed immediately by decay by proton emission. The effect is likely to be very small and again only important above 18MeV.

O16

CONSISTENCY PROBLEM

We processed JEF2 to get point heating. Ziver(6) has used JENDL. The JENDL data were examined but JEF2 seemed better. The JENDL3.1 data were also processed and compared.

Graphical and percentage differences in point heating were produced. Below 0.0253eV JENDL3.1 was about 40% higher. The difference then steadily decreases with increasing energy until 0.5eV when coincident values are seen. By 3.6eV JEF2.2 point heating has become about 3% higher where it remains until about 80KeV. Between 80KeV and 4.8MeV there is fluctuation but differences are usually less than 10%. Between 4.8 and 13MeV JEF is generally higher by up to a factor of 2. Above 13MeV JENDL data are higher by up to a factor 3.

In general the JEF2.2 gamma production data seems to be backed by experimental results whereas the JENDL3.1 is based on theoretical results. It would thus seem better to use the JEF2.2 evaluation.

The comments below refer to JEF2.

There are no continuous photon energy spectra for O16. (MF=15) All gamma lines are described within multiplicities (MF=12) and photon production cross sections (MF=13).

Level 1 decays by electron/positron pair production. (LR=40) and is mentioned on pages 0.26 and 0.27 of BNL-NCS 44945. (14)

It seems this leads to a pair of gamma rays:-

```
****NOTE THAT THE FIRST EXCITED LEVEL OF O16 AT 6.052 MEV IS      825 1451 191
****ASSUMED TO DECAY WITH EMISSION OF TWO 0.51 MEV GAMMA RAYS    825 1451 192
```

These are the only gamma rays emitted from the level. The multiplicity increases to 2.046 at 20 MeV incident energy. It seems from the HEATR print that this unusual reaction is processed correctly to get the remaining point heating.

Again dummy inelastic levels have been used. Comments note:-

```
****PLEASE NOTE THAT MUCH OF THE CROSS SECTION TO LEVELS ABOVE 825 1451 109
****9 MEV SUBSEQUENTLY RESULTS IN CHARGED PARTICLE EMISSION.      825 1451 110
****MT=56-58,61-66,68-70,72-73,75,77-78,80,82-83,85,87,89, ARE 825 1451 111
****FLAGGED AS DECAYING BY ALPHA EMISSION. THIS CHOICE LEADS T 825 1451 112
****A TOTAL ALPHA EMISSION X/S SIMILAR TO DATA OF LI52,DA68,BO6 825 1451 113
****BELOW 17 MEV. THE REMAINING MT NUMBERS ABOVE MT=66 ARE      825 1451 114
****FLAGGED AS BEING PROTON EMITTERS.                             825 1451 115
```

similar effects to those mentioned for Al27 will be seen.

The (n,alpha) reaction is split into cross sections for the various ground and metastable states of 13C. This is done using reactions Mt=800-803. (ENDF5 used MT=780-783).

The comments on the cross section are:-

```
MT=107 (N,ALPHA) CROSS SECTION                                     825 1451 131
  THRES. TO 20 MEV, SUM OF MT=780-783.                          825 1451 132
                                                                825 1451 133
MT=800 (N,ALPHA) INTEGRATED CROSS SECTION TO 13C GROUND STATE 825 1451 134
  0.0 TO 6.2 MEV, BASED ON R-MATRIX ANALYSIS DESCRIBED ABOVE    825 1451 135
  UNDER MT=1. ENERGY SCALE OF BA72 ADJUSTED TO                825 1451 136
  MATCH TOTAL CROSS SECT AND RESOLUTION CORRECTIONS APPLI-     825 1451 137
  ED TO GIVE WIDTH AND HEIGHT OF PEAKS CONSISTENT WITH         825 1451 138
  TOTAL. NORMALIZATION OF 0.808 FOR BA72 DETERMINED FROM       825 1451 139
  R-MATRIX FIT AND APPLIED. LEVEL SCHEME DETERMINED FROM      825 1451 140
  R-MATRIX ANALYSIS AND SE86.                                    825 1451 141
  6.2 TO 20 MEV, BASED ON DATA OF DA63, DA68, SI68, BA73, AND 825 1451 142
  COMPOSITE OF MC66A, MA68, AND LE68 AT 14 MEV. NOTE THAT     825 1451 143
  THE DA63 DATA WERE RENORMALIZED BY FACTOR OF 1.7 TO         825 1451 144
  BRING THEM INTO ROUGH AGREEMENT WITH THE R-MATRIX ANALYSIS 825 1451 145
  OF THE BA73 (N,A0) DATA, TOGETHER WITH THE TOTAL AND        825 1451 146
  ELASTIC DATA IN THE ANALYSIS. BECAUSE THE DA68 EXP. DATA 825 1451 147
  WERE NORMALIZED TO DA63, THE FORMER WERE ALSO RE-           825 1451 148
  NORMALIZED BY THE FACTOR OF 1.7.                              825 1451 149
                                                                825 1451 150
MT=801-803 (N,A) CROSS SECTION TO EXCITED LEVELS OF C13.     825 1451 151
  THRES. TO 15 MEV, USED (N,A) DATA OF DA63 AND SI68, AND THE 825 1451 152
  (N,AG) DATA OF NE90, NO78, DI70, OR70, CL69, NY69, EN64,   825 1451 153
  AND BU71.                                                     825 1451 154
```

NJOY treats the component cross sections MT=800 -803 rather than the total MT=107.

This caused NJOY89.62w to fail in HEATR with the message:-

```
***error in findf***mat 825 mf 4 mt800 not on tape 13.
***fatal
```

This is saying there are no angular data describing the emitted alphas. As there are rarely angular distributions for particles other than neutrons in MF 4, it seems the NJOY89.62w test was probably defining MT=800 as emitting neutrons! In a test isotropic data were added in MF=4. The code then failed because the UNRESR module had corrupted one of the Q values on the PENDF with the broadened temperature!

NJOY91.76 includes corrections which allow processing of this reaction. The JEF steering committee recommend the use of NJOY89.62 unless processing is incorrect. Then NJOY91 can be used given that the use of NJOY91 is noted. NJOY91.76w was used.

Si

The comments note that there are level data for (n,p) and (n,alpha) specified.
 MF 600 - 614, 649 for (n,p) levels and continuum.
 MF 800 - 811, 849 for (n,alpha) levels and continuum.
 Thus NJOY91.76w was used (see O16 above) without problem.

Zr

There is negative point heating in HEATR output at 2MeV thus:-

		low
min	1.0363E+05	
2.0000E+06	-6.8137E+05	
max	1.0485E+05	

Inelastic levels terminate at 2MeV and continuum inelastic threshold is at this energy. The continuum data are:-

2.000000+6 0.000000+0 2.000100+6 5.950000-1 3.000000+6

Total inelastic (MT=4) are:-

1.900000+6 5.646670-1 1.950000+6 5.800000-1 2.000100+6 5.950000-14000 3 4 492
 3.000000+6 1.190000+0 4.000000+6 1.550000+0 5.000000+6 1.600000+04000 3 4 493

By terminating the levels at 2MeV the evaluator created a dummy valley between 2 and 2.0001 MeV. However the levels are terminated correctly by specifying two energies at 2 MeV; the first with the correct cross section and the last with zero cross section. This procedure is defined on page 3.2 and 3.3 of BNL-NCS 44945 (14) It seems the HEATR module of NJOY defines the heating at the last point. Hence the total heating at 2MeV from the levels is zero. The gamma production cross section is continuous around 2MeV thus:-

9.300000+5 0.000000+0 1.000000+6 1.845200-1 1.500000+6 1.029700+0400013 31332
 2.000000+6 1.668700+0 4.000000+6 3.925700+0 6.000000+6 4.657100+0400013 31333

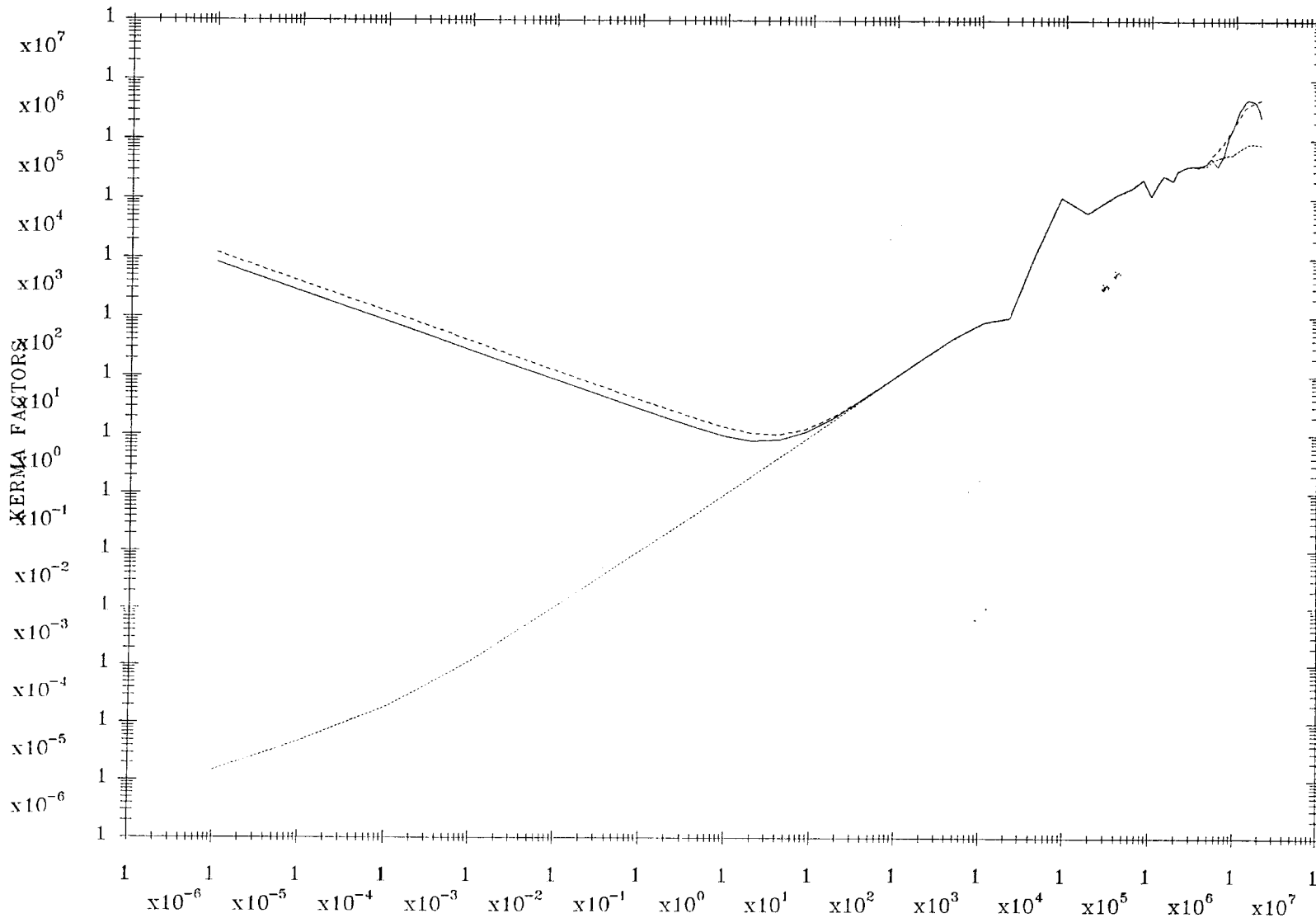
Hence the gamma energy release is subtracted from the zero total to give the negative heating seen. 2Mev is the boundary between groups 460 and 461 in the GROUPT output. There are no negative group heating data or noticeable changes in values:-

451	9.898E+04
452	1.171E+05
453	1.231E+05
454	1.147E+05
455	1.153E+05
456	1.121E+05
457	1.290E+05
458	1.171E+05
459	1.254E+05
460	1.307E+05
461	2.631E+05
462	2.908E+05
463	3.179E+05
464	3.451E+05
465	3.722E+05
466	3.989E+05
467	4.252E+05
468	4.515E+05
469	4.777E+05
470	5.040E+05

The JEF2.2 inelastic data are taken from ENDL78 and are unchanged in ENDL84. The high energy isotopic data are not consistent but the isotopic evaluations contain no gamma source data. There are no gamma source data in ENDF/B-VI for natural Zr or Zr isotopes. It may be worth considering the JENDL3.1 natural Zr data if total heating in Zr is found to be poor. However any decision to change requires both point and gamma heating to be altered and preferably the cross sections. The resonance data in JEF2.2 seem to have been chosen with care and a full study of all aspects is required before using JENDL3.1.

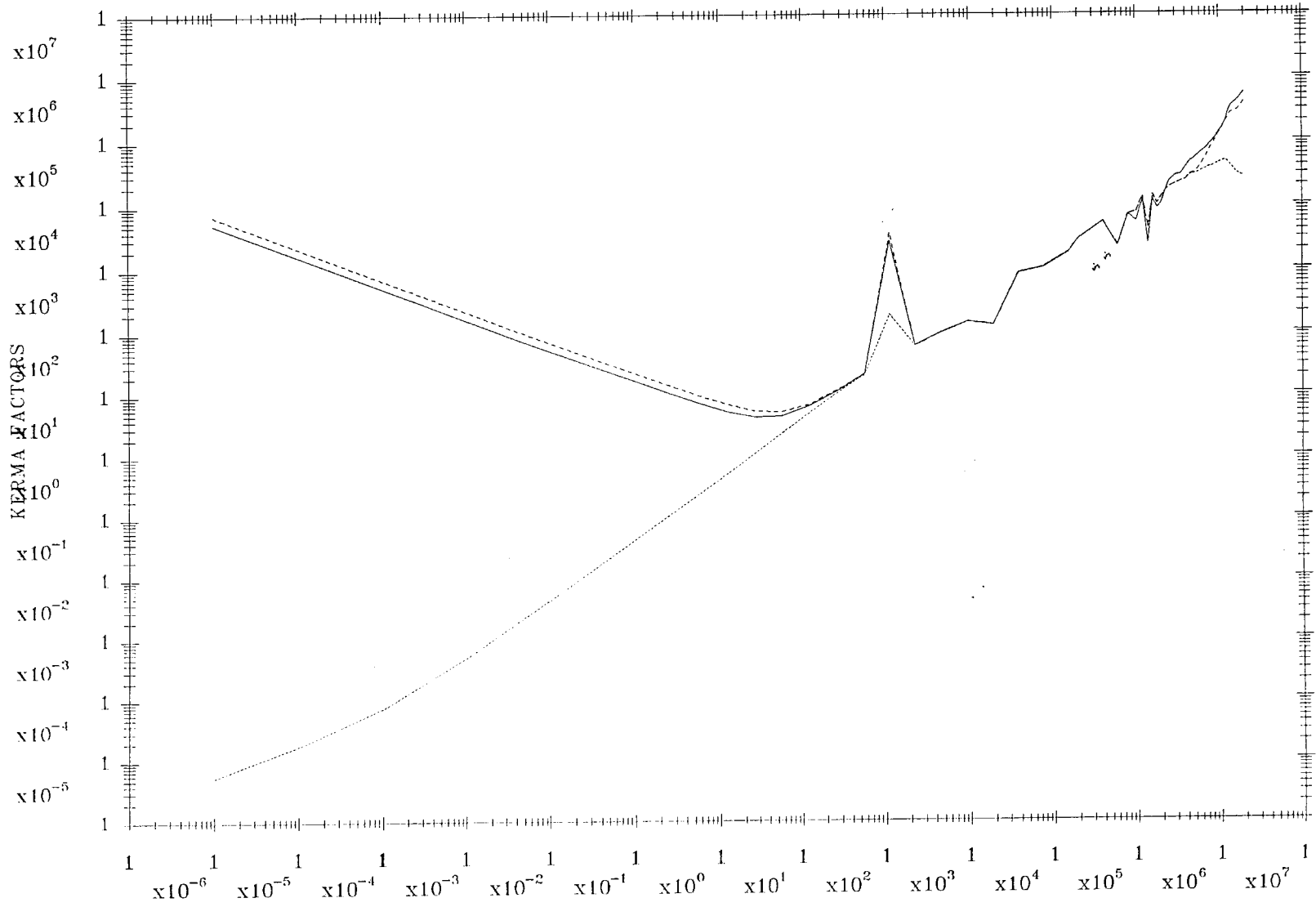
Al27 Kerma

FINAL KERMA FACTORS - Al27 - NJOY89 - JEF2.2



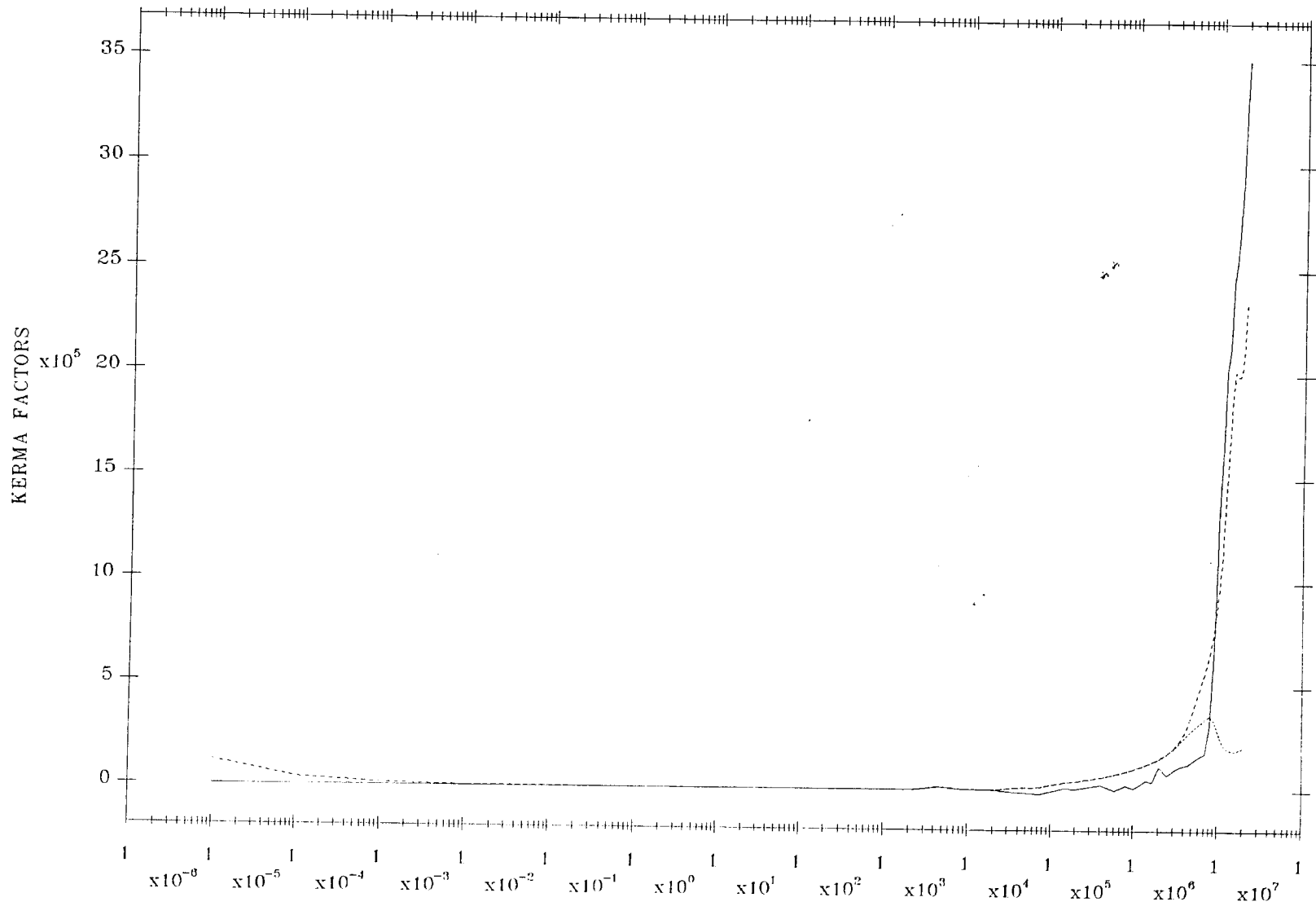
Fe56 Kerma

FINAL KERMA FACTORS - Fe56 - NJOY89 - JEF2.2



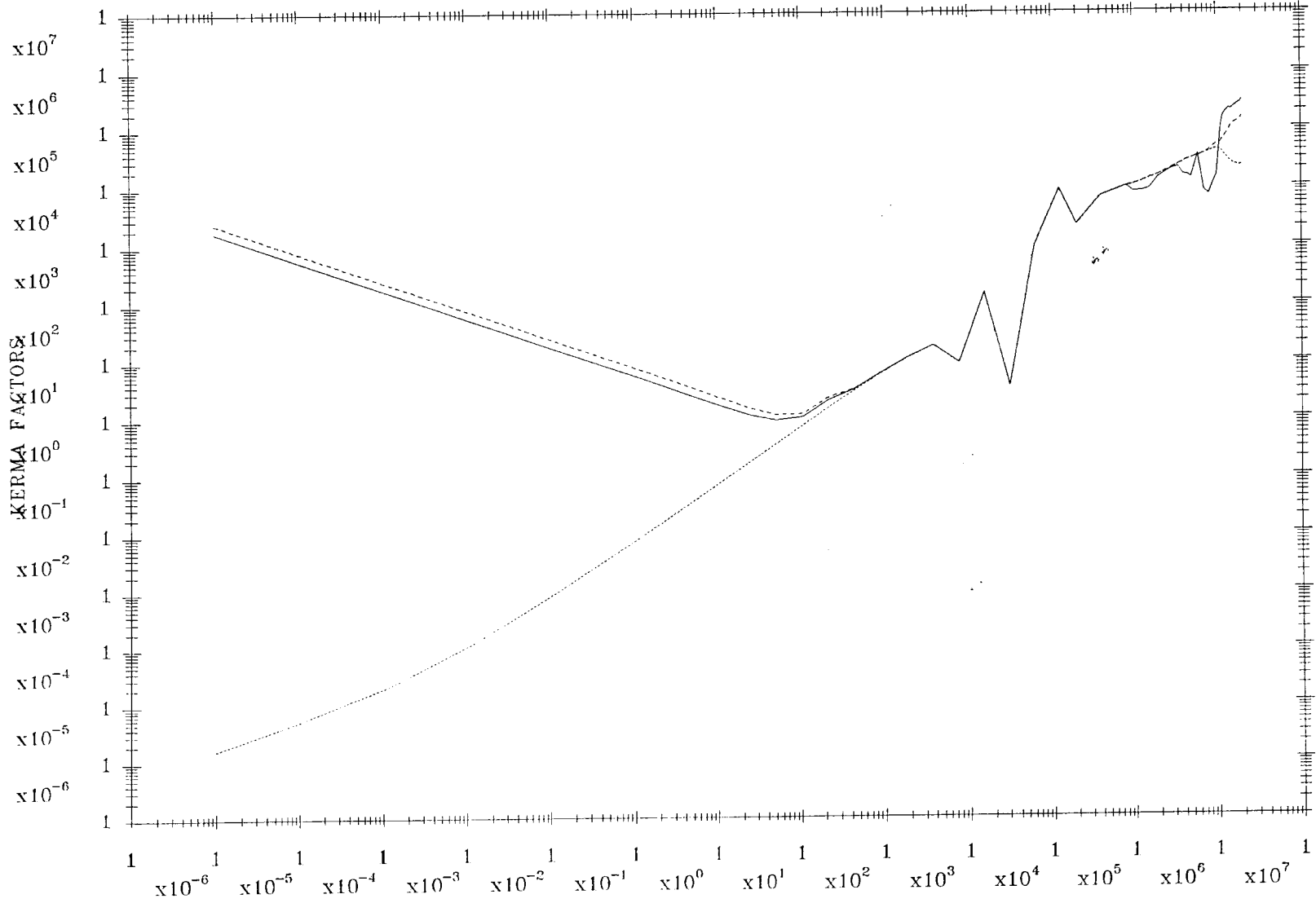
Fe57 Kerma

FINAL KERMA FACTORS - Fe57 - NJOY89 - JEF2.2



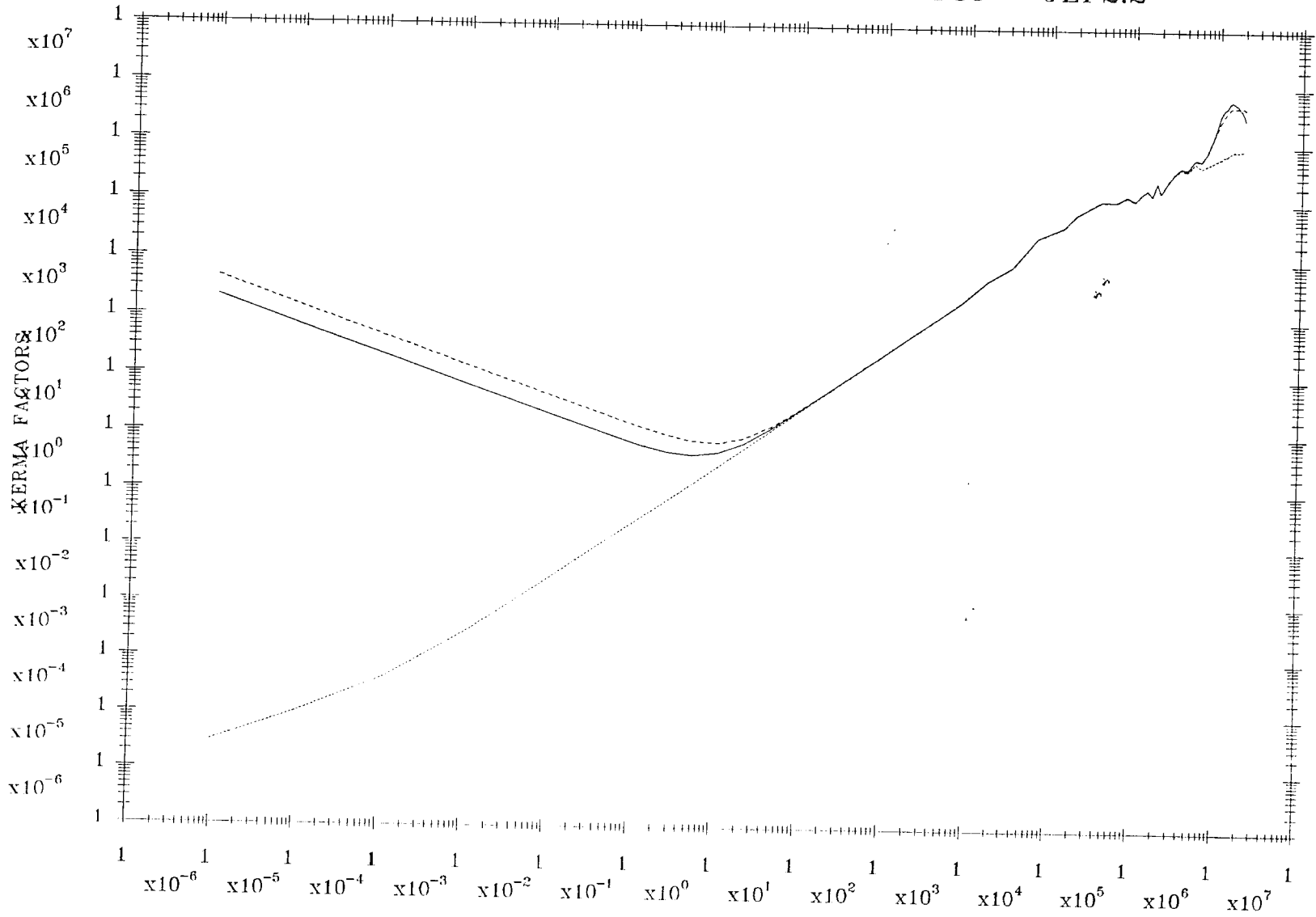
Fe58 Kerma

FINAL KERMA FACTORS - Fe58 - NJOY89 - JEF2.2



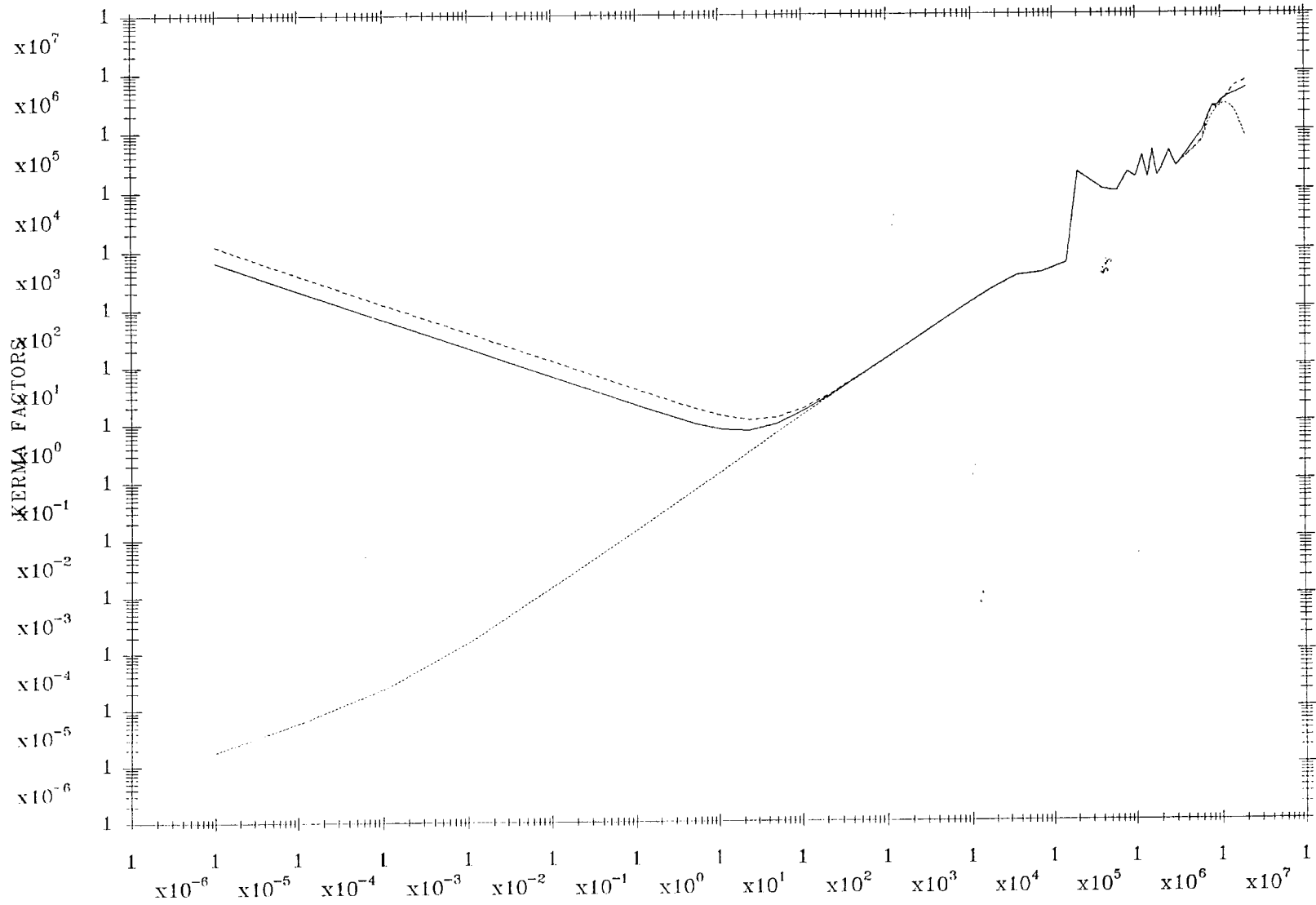
Mg Kerma

FINAL KERMA FACTORS - MG - NJOY89 - JEF2.2



Si Kerma

FINAL KERMA FACTORS - Si - NJOY91 - JEF2.2



Zr Kerma

FINAL KERMA FACTORS - Zr - NJOY89 - JEF2.2

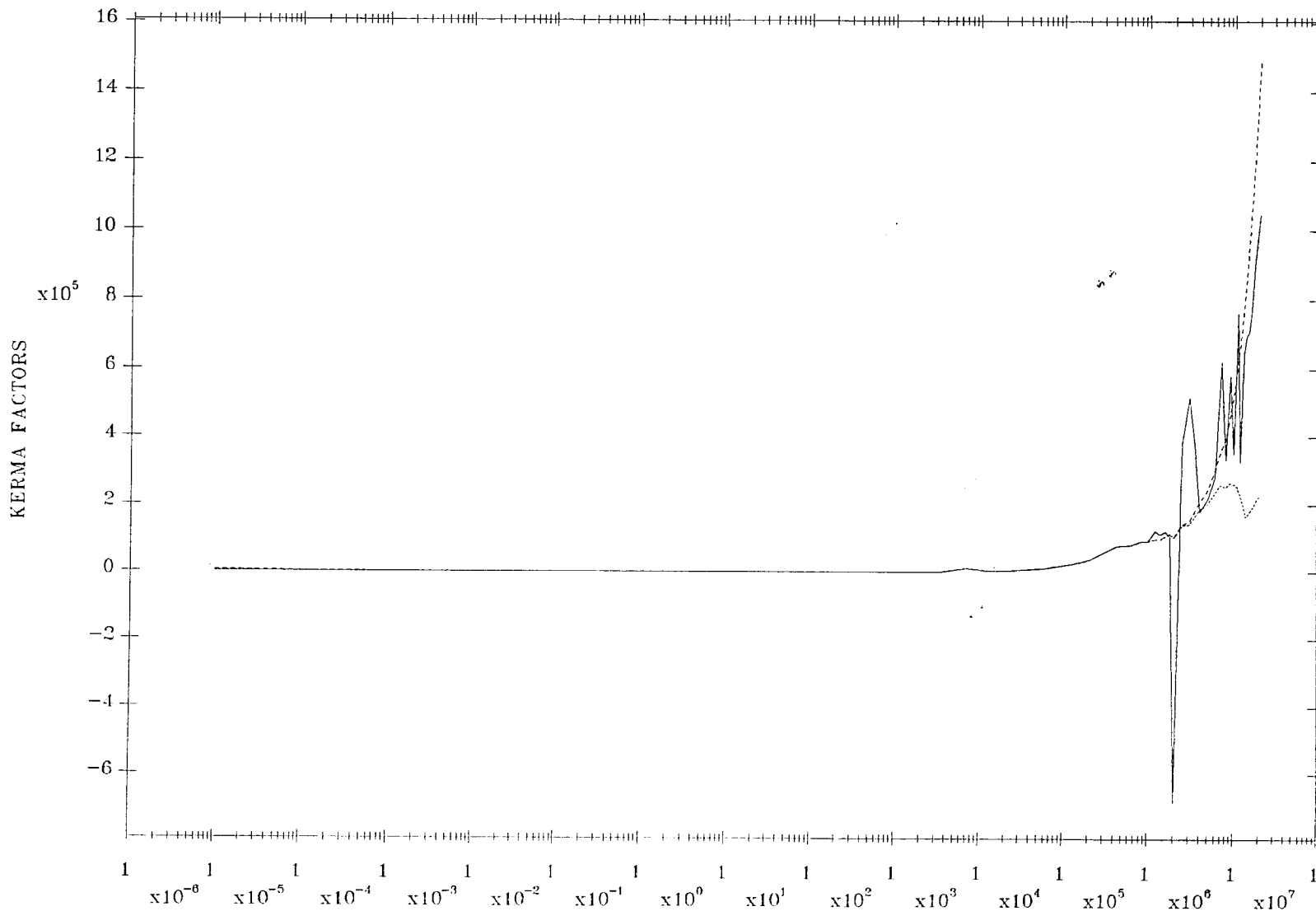


Table 5 : Shielding effects (Maximum Differences)

Al27 77% difference at 5.75 KeV

C 10% difference at 2.9 MeV

Ca 45% difference at 425 KeV

Fe54 96% difference at 69 KeV

Fe56 93% difference at 72KeV and 80KeV

Fe57 1329% difference at 180KeV (Note negatives!!)

Fe58 82% difference at 230KeV

H1 (negligeable)

O16 18% difference at 2.3 MeV

Mg 9% difference at 840 KeV

Si 18% difference at 1.2 MeV

Zr 73% difference at 2.55 KeV

Appendix 5. Processing Unresolved Resonances in Fe56 Evaluations

The JEF2 evaluation for Fe56 contains resolved resonance parameters up to 862KeV. Unresolved parameters are given up to 3MeV. However the LSSF flag is set to 1 indicating that the infinitely dilute cross section in the range 862KeV - 3MeV is completely described in the file 3 data (tabulated cross sections). Normally LSSF=0 and cross sections generated from file 2 resonance parameters must be added to background cross sections given in file 3.

Examination of the file 3 Fe56 data seems to indicate cross sections for inelastic to the first level contain some fluctuations but not detailed enough to be consistent with the presence of a statistical ladder generated from unresolved parameters. The total contains more detailed fluctuations which seem to fully describe the structure (although the energy grid indicates poor resolution). The relatively small capture contains no significant structure. Elastic has been formed by subtracting inelastic and capture from total. Elastic and inelastic data are graphed across the join between resolved and unresolved parameters in figures A5.1 and A5.2. The smoothly varying elastic data below 862KeV can be contrasted with the lack of points above. However there seem to be a similar number of resonances present. The inelastic seems only to represent two resonances which are rather broad!

The ENDF/B-VI (revision 1) file for Fe56 contains resolved resonance parameters up to 850KeV. However it has no unresolved parameters. Similar fluctuations are present in inelastic, elastic and total but again not in the small capture cross section. The capture is however about twice the JEF2.2 value. Elastic and inelastic data are graphed across the join between resolved and unresolved parameters in figures A5.3 and A5.4. The smoothly varying elastic data below 850KeV can be contrasted with the lack of points above. There also appears to be a problem in resonance valleys. Again there seem to be a similar number of resonances present. The inelastic seems only to represent two resonances which are rather broad. The first resonance has been "executed".

The two sets of data are probably taken from the same source with slightly different processing (problems) applied.

Processing of Cross Sections

When shielded cross sections are required the UNRESR module of NJOY is run. For the JEF2.2 Fe56 evaluation, UNRESR generates data at two incident energies from the resonance parameters. At 862 KeV and 1 MeV it forms infinite dilute and shielded data for total, elastic, fission, capture and transport (No inelastic or heating). THERE IS A 1MEV CUT OFF SO NO SHIELDED DATA FOR FE56 ARE GENERATED IN THE RANGE 1 - 3 MEV. These data

are added in section 2 of the PENDF. Section 3 of the PENDF contains infinite dilute cross sections processed from the file 3 of the JEF2.2 file by Doppler broadening and transferring to a unified energy grid (the BROADR module of NJOY). The resonance parameters are ignored when generating these data because the LSSF flag is set to 1. GROUPR picks up the file 3 data and corrects using the file 2 data thus:-

```
if (lssf.eq.0) sig(is)=sig(is)+s-sinf          GROUPR 03421
if (lssf.gt.0.and.$inf.ne.0.0) sig(is)=sig(is)*s/sinf    MAR91W 00012
```

where the right hand side terms are:-

sig(is) the file 3 cross section,

s the file 2 shielded cross section,

sinf the file 2 infinite dilute cross section,

remembering that lssf=1 for JEF2 Fe56.

The status of processing unresolved resonance data was summarised by Rowlands (30) in 1984. The comments in this appendix indicate very little has changed in practice. There are hopefully improvements in the release of the PURR module in NJOY91.76w. Ribon's CALENDF code (31) has been used to generate ECCO (32) data and work is underway with a modern version of GENEX (33). A coordinated approach is required so that improvements in evaluations remain consistent with whichever of these methods are used by processors.

Heating

The HEATR module of NJOY has no knowledge of the requirement for totally shielded heating. Thus there is no scaling of the infinite dilute data in the unresolved range before integrating over the groups. This means heating is generated as though the file contained no unresolved parameters. ie it is rather like the ENDF/B-VI evaluation. A comment in BNL-NCS-17541(9) page 154 notes that Fe56(n,n') exciting the 0.847MeV level up to 5MeV is known to 5-10% but is required to 2% for pressure vessel surveillance. It is thus also important to shield and process this region correctly to obtain damage rates which are closely related to heating. At present we are probably generating heating data to within the accuracy of the current evaluated data.

Conclusions

- 1 The Fe56 evaluations in JEF2.2 and ENDF/B-VI should be reviewed and the problems described above explained.
- 2 The 1MeV cut off in the UNRESR module of should be replaced by the top energy of the evaluation's unresolved resonance region.

Better methods of processing unresolved data should be fully incorporated in NJOY.

Figure A5.1. JEF2.2

Resolved Resonances to 862 KeV

A.48

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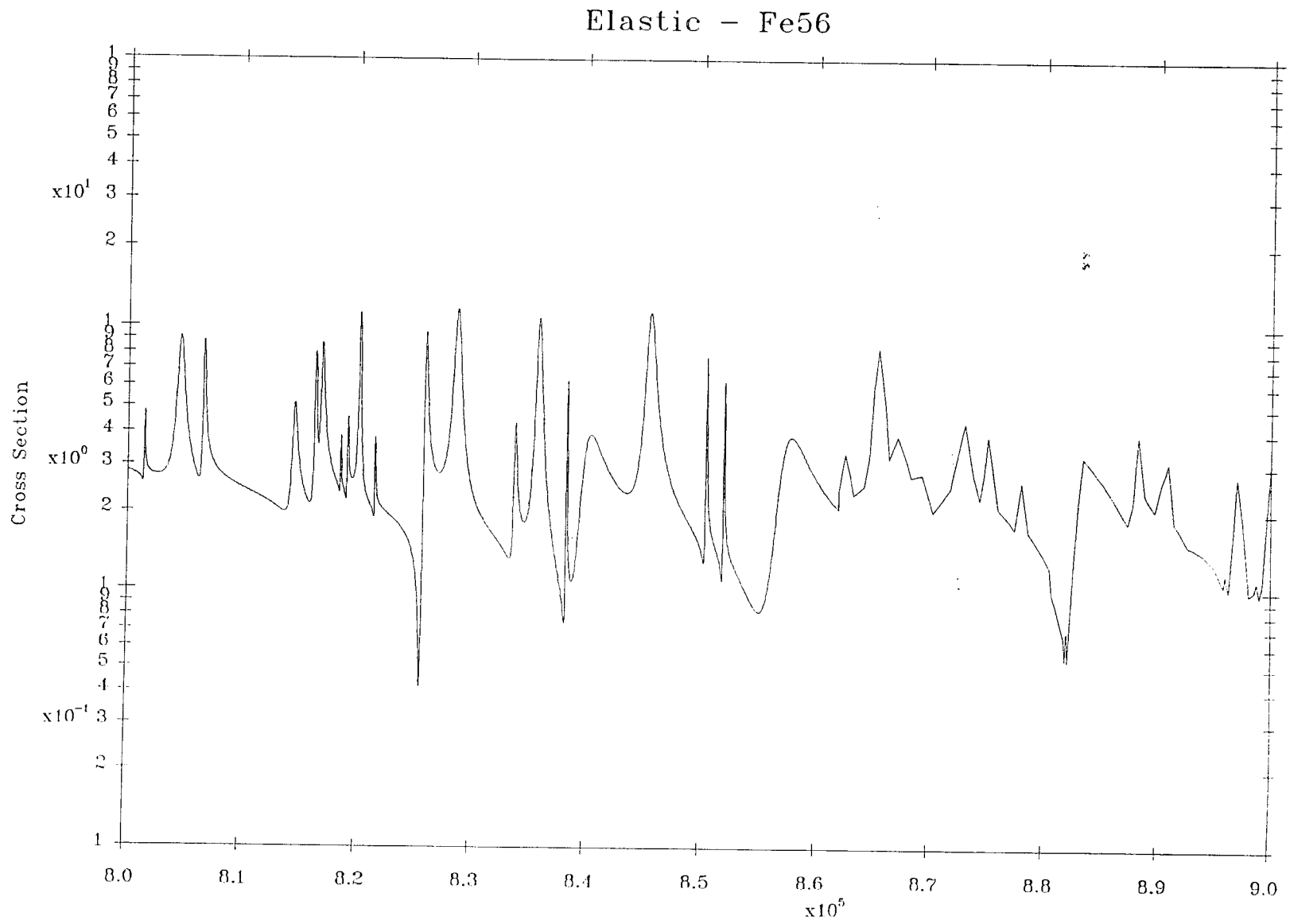


Figure A5.2. JEF2.2

Note the lack of Structure compared with Elastic (Figure A5.1)

A.49 AEA Technology

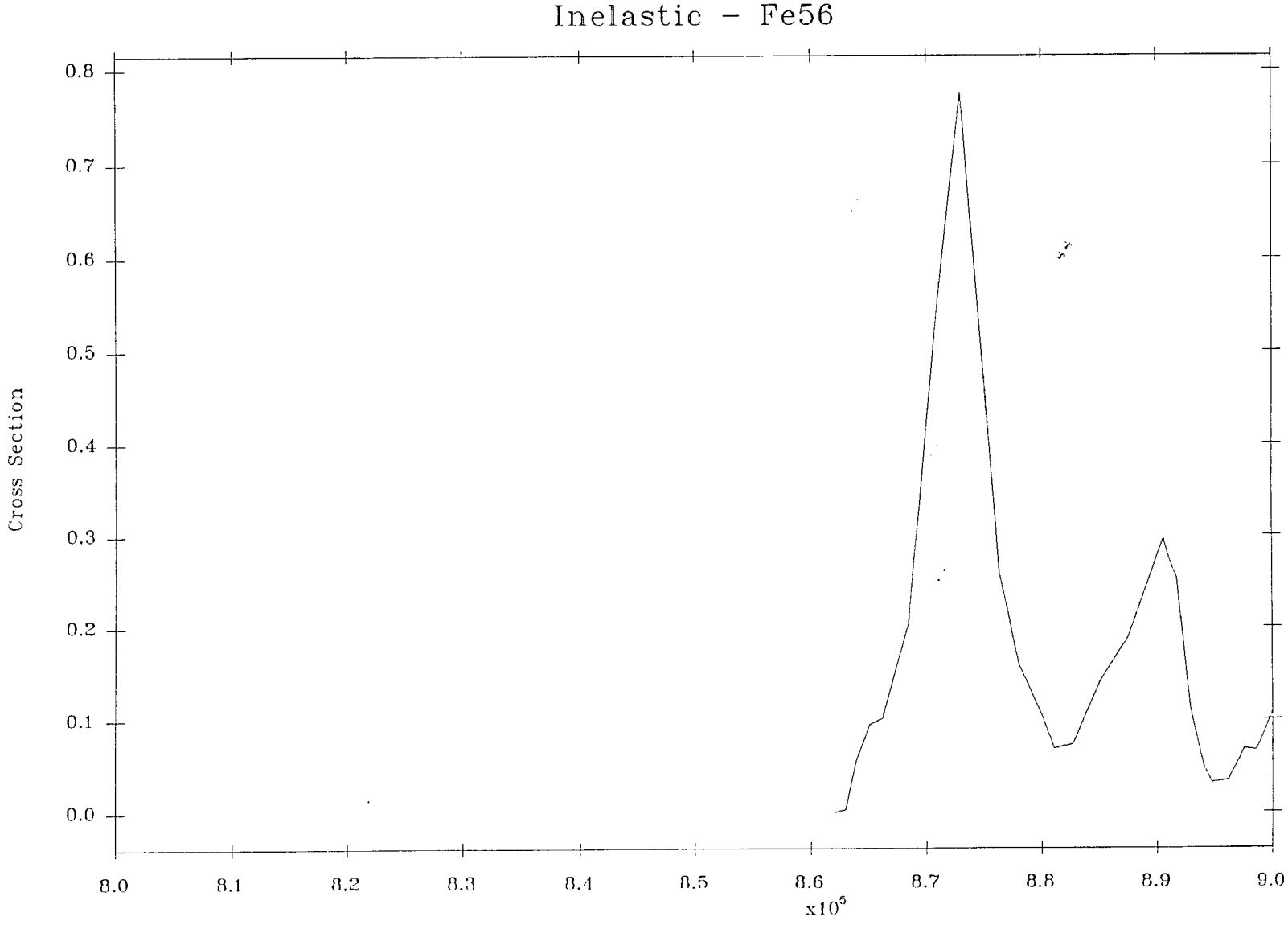


Figure A5.3. ENDF/B-VI

Resolved Resonances to 850 KeV

A.50
AEA Technology

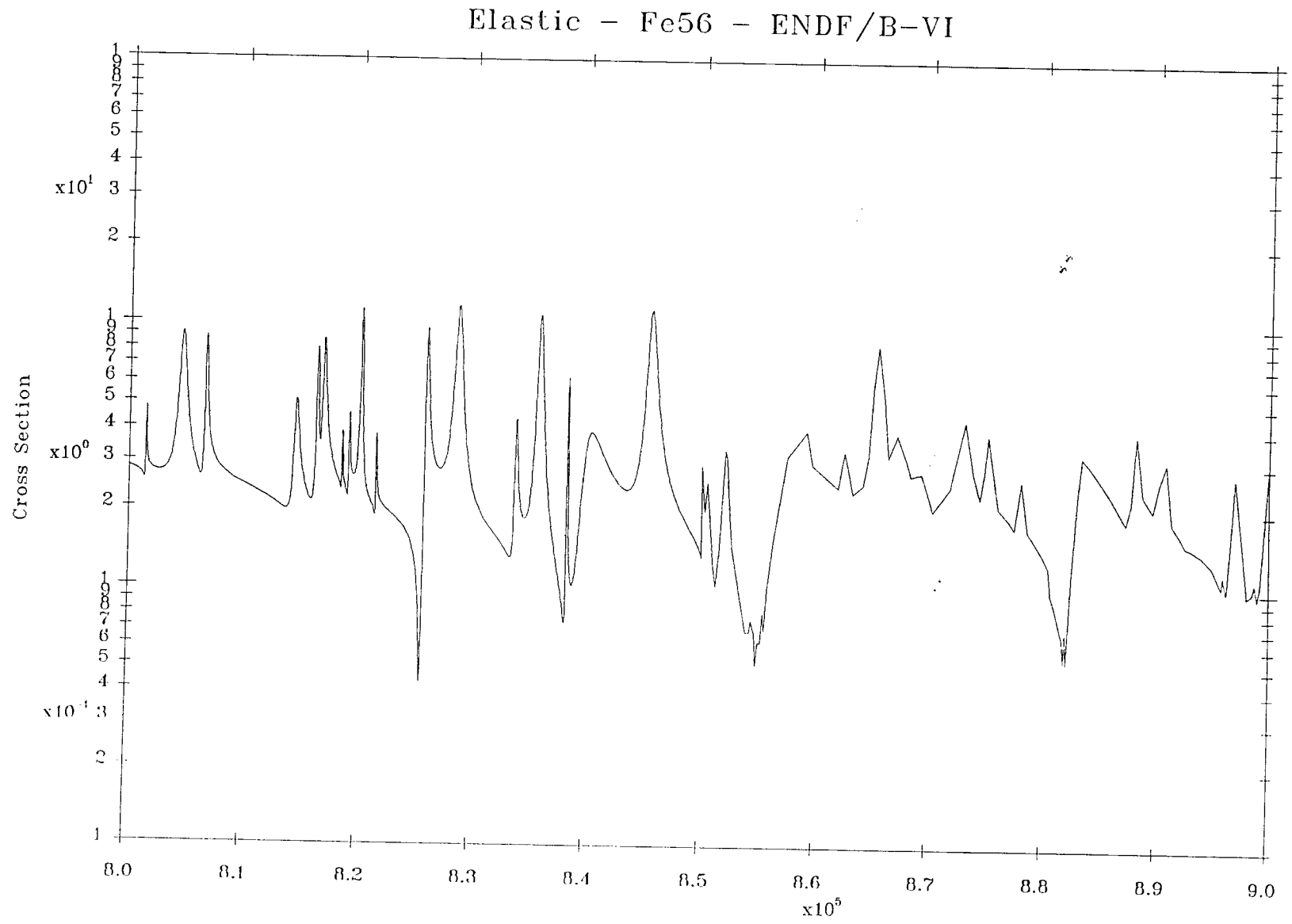


Figure A5.4. ENDF/B-VI

Note the lack of structure compared with Elastic (Figure A5.3)

A.51
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Inelastic - Fe56 - ENDF/B-VI

