PROCESSING AND TESTING ENDF/B-VI WITH NJOY AND TRANSX

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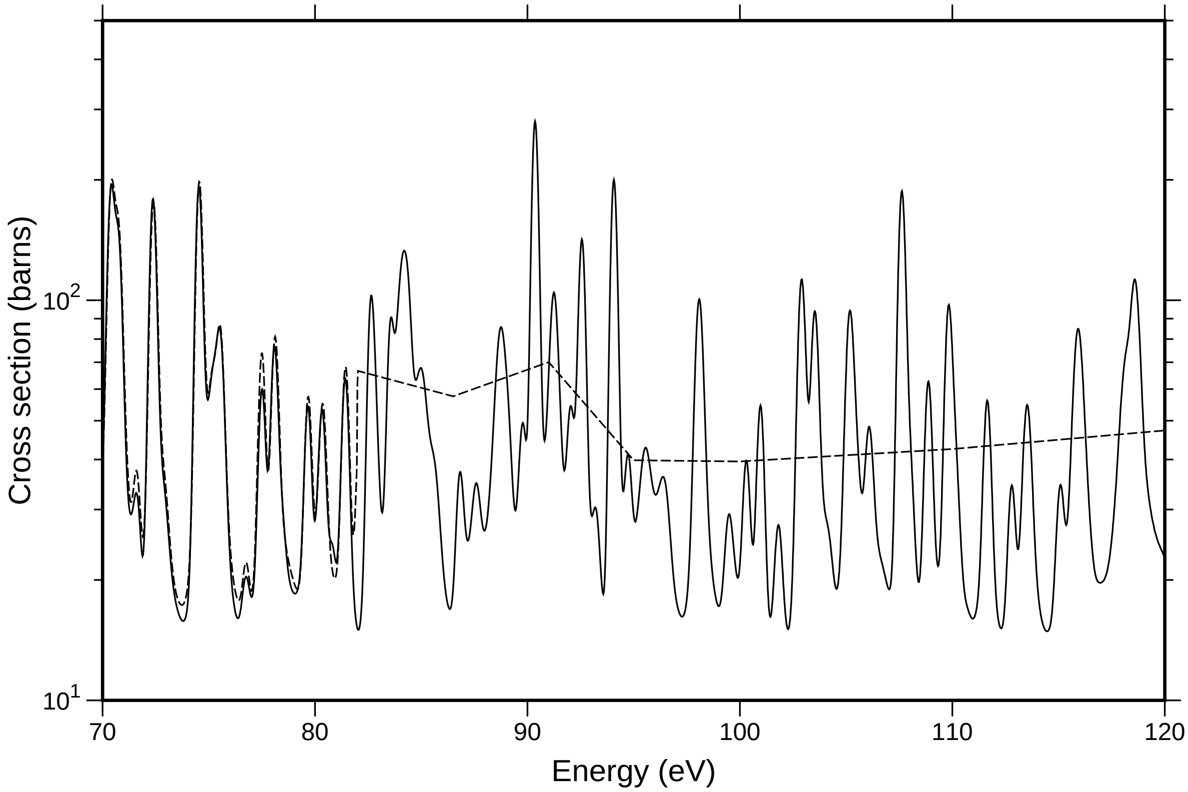
INTRODUCTION

- The NJOY Nuclear Data Processing System has been used to process ENDF/B-VI for multigroup and Monte Carlo libraries.
- New features of the ENDF-6 format
- Code modifications to handle the new evaluations
- Testing of code and data

ENDF/B-VI FEATURES

The ENDF/B-VI files contain a number of new features of interest to reactor physics:

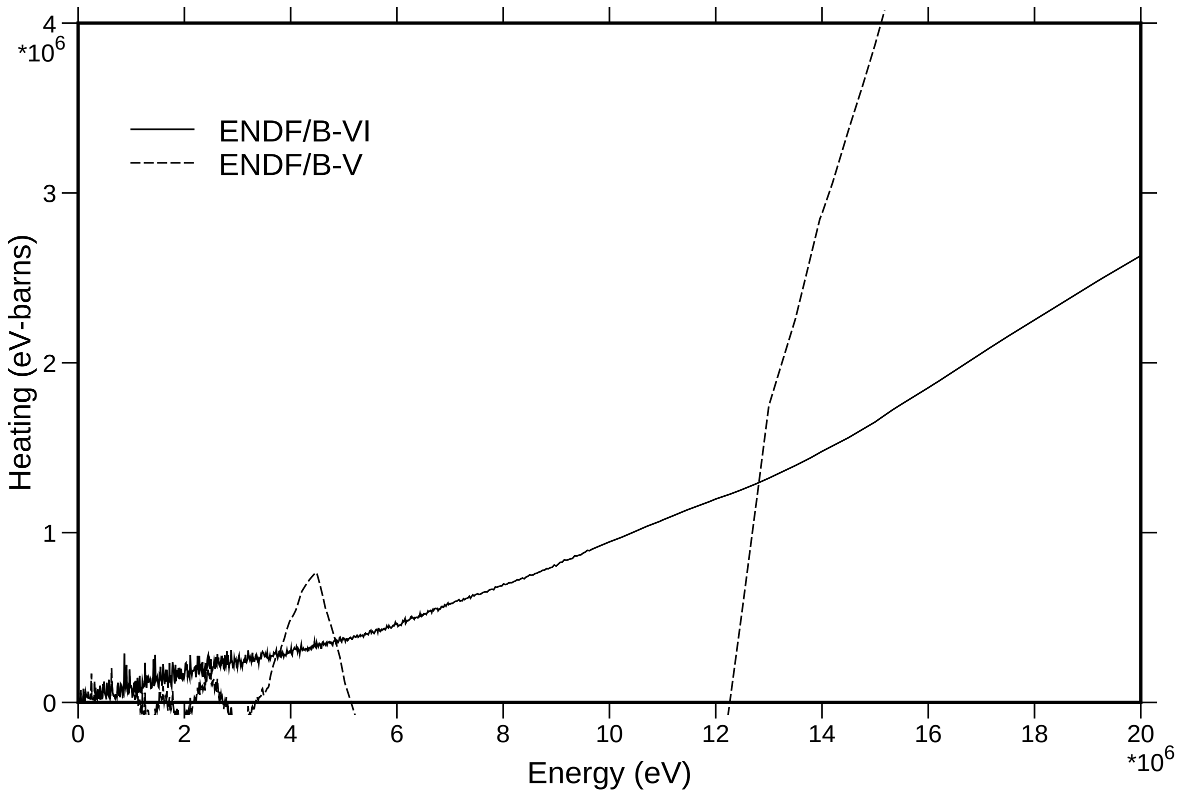
- ^{235}U, ^{238}U, and ^{239}Pu extended resonance ranges
  - ^{235}U: 82 eV extended to 2.25 keV
  - ^{238}U: 4 keV extended to 10 keV
  - ^{239}Pu: 300 eV extended to 1 keV
- Reich-Moore resonance parameters
  - Actinides
  - Structurals (Fe, Ni, Cr, Cu, Pb)
  - Better line shapes
  - No backgrounds
- Energy-angle distributions
  - Better high-energy transport
  - Better KERMA and damage



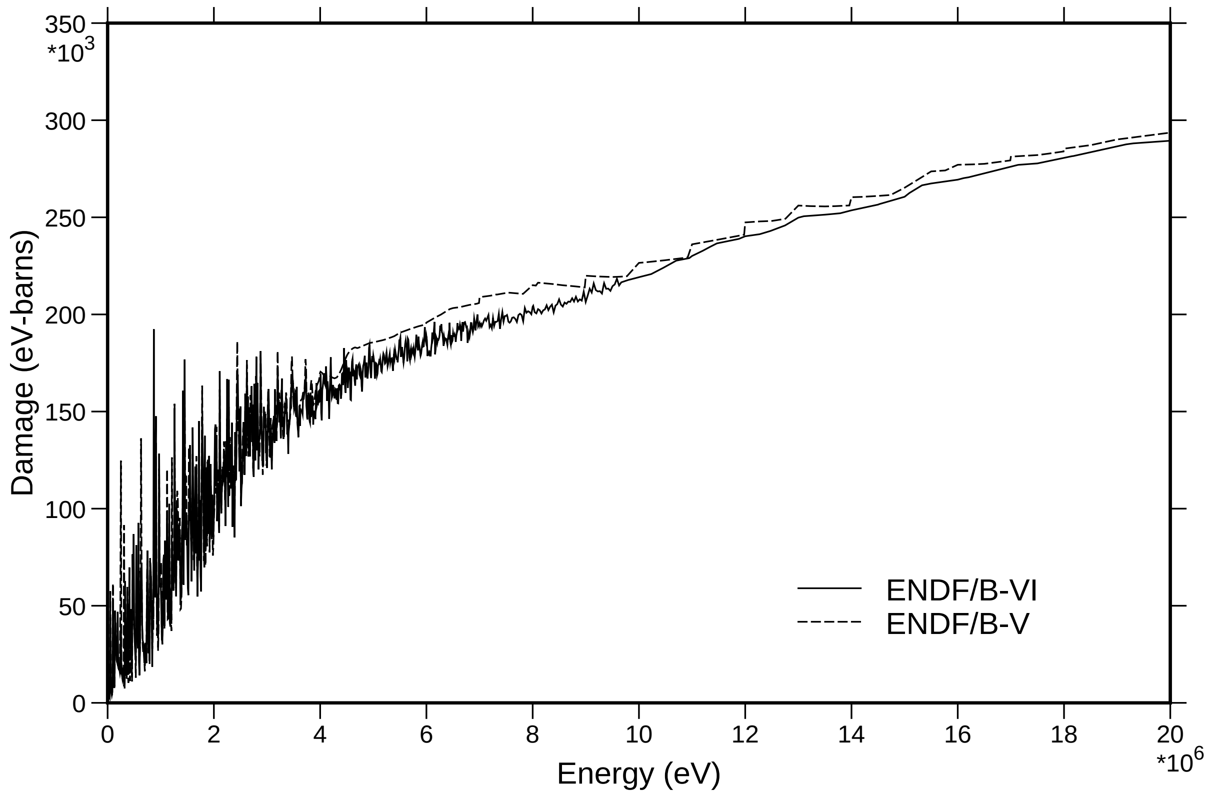
Total cross section for ^{235}U showing that part of the range that was given as unresolved in ENDF/B-V (dashed) is well resolved in ENDF/B-VI (solid).

FILE 6 BENEFITS FOR HEATING AND DAMAGE

- Isotopic evaluations are given.
- Explicit energy-angle distributions are given for emitted charged particles and recoil nuclei.
- Heating and damage can be computed directly without recourse to energy-balance arguments or built-in reaction models.
- ENDF/B-V required: *CP Energy* = *Available Energy* − *Neutron Energy* − *Photon Energy*.



KERMA comparison for chromium



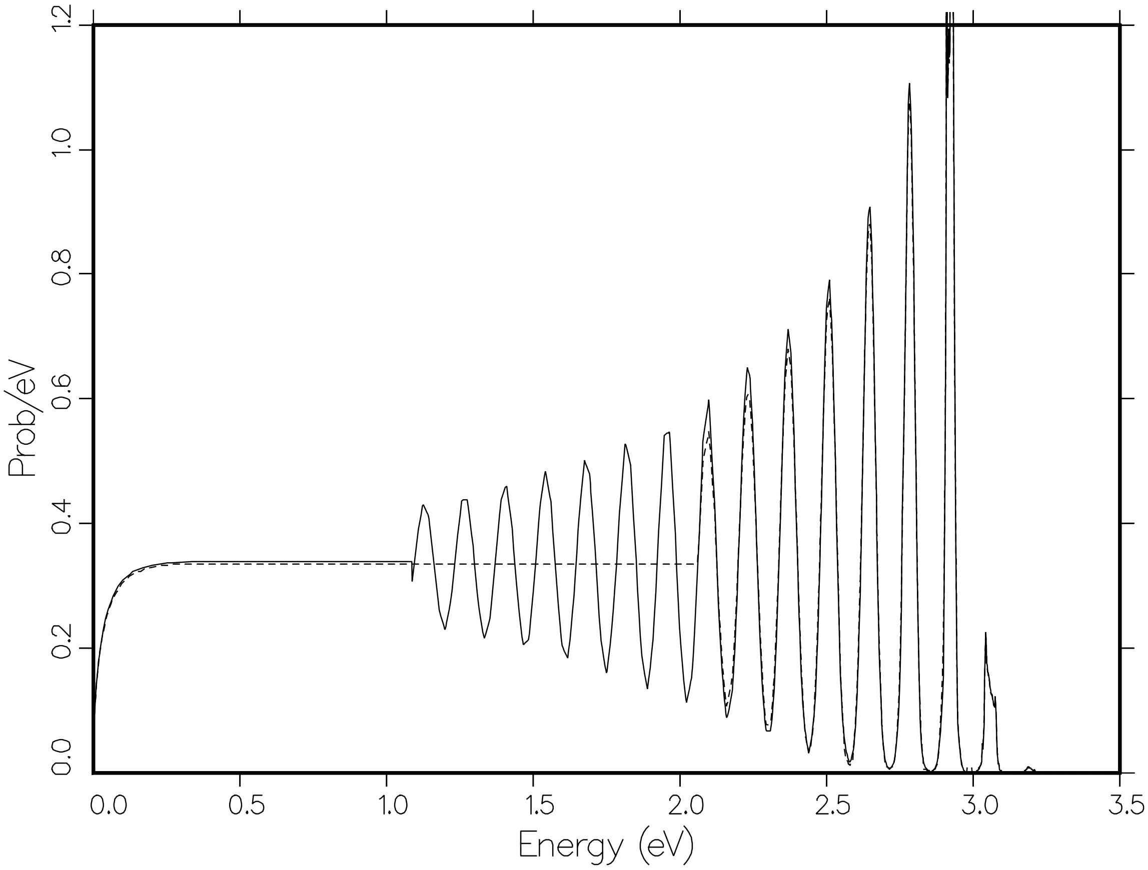
Damage comparison for chromium.

FILE 6 BENEFITS
FOR TRANSPORT

- Coupled energy-angle distributions for secondary neutrons and outgoing particles in "File 6"
  - Kalbach systematics (LANL)
  - Legendre distributions in lab (ORNL)
  - Angle-energy distributions in lab (LLNL)
  - Phase-space distributions (LANL)
- Important for fusion and shielding applications
- Effects for fission-reactor problems remain to be evaluated.

THERMAL CHANGES

- File 7 format changes
- Conversion of old ENDF/B-III evaluations originally prepared by GAB.
- New LANL evaluations to improve accuracy and extend energy range using GA models.



Neutron spectrum from H in ZrH for an energy of 3.059 eV. The solid curve is for the new evaluation, and the dashed curve is for the older evaluation.

NJOY DEVELOPMENT

- NJOY has been gradually upgraded to handle the new features of the ENDF-6 format.
- This effort has been aided by users at other laboratories in the US and around the world.
- Much of the coding to handle the new resonance options was provided by Dunford (NNDC).
- Resonance reconstruction was tested by an international effort (IAEA, NEA Data Bank, ORNL).
- The File 6 energy-angle work as done was at Los Alamos
  - HEATR module to compute heating and damage
  - GROUPR module to compute multigroup transfer matrices for emitted neutrons, charged particles, and photons
  - ACER module for producing MCNP libraries (cooperation between T-2 and X-6).
- Latest steps consisted of getting NJOY and MCNP to work together properly for ENDF/B-VI data.
  - MCNP4A released.
  - Legendre distributions as used by ORNL are currently approximated by converting them to Kalbach form for sampling.

PROCESSED LIBRARIES

- NJOY 91.91 was used to process many of the materials of ENDF/B-VI.2 into several multigroup libraries in MATXS format.
  - MATXS10 is a 30x12 library that is compact and useful for high-energy problems where resonance effects are not important.
  - MATXS11 is an 80x24 library with extensive self-shielding tables useful for fast-reactor and fusion studies.
  - MATXS12 is a 69x24 thermal reactor library with self-shielding and upscatter (250 materials, including fission products).
  - MATXS13 is a 187x24 multipurpose library for fusion, fast-reactor, and thermal-reactor problems.
  - MATXS14 is a 175x42 library for fusion neutronics studies.
  - ENDF/B counterparts: MATXS5, MATXS6, MATXS7, MATXS8.
- ACE-format library for MCNP (125 materials).

These cross section libraries will soon be available from the Radiation Shielding Information Center (RSIC) at Oak Ridge.

DATA TESTING

An important part of the release of each new version of the ENDF/B libraries has been testing:

- Testing for proper use of the formats
- Testing the physical consistency of the data in the files
- Testing against selected benchmarks

CONSISTENCY TESTING
ENERGY BALANCE

As part of the consistency testing, we have performed a detailed energy-balance study of ENDF/B-VI:

- ENDF/B-VI is overall a great improvement over ENDF/B-V, especially for the important structural materials Fe, Ni, Cr, and Cu.
- There are still problems (including negative KERMA factors)

Energy-Balance Problems for ENDF/B-VI:

Summary of the materials that need the most improvement for the thermal range, fission range (.1 to 2 MeV), and fusion range (2 to 20 MeV). The entries in the thermal column have errors in photon energy production from 1 to 22%. The entries in the other two columns have negative KERMA values, values greater than twice the kinematic maximum, or values less than half of the kinematic minimum. Most of these materials were carried over from earlier ENDF/B versions.

Thermal	Fission	Fusion
17-Cl-nat	42-Mo-nat	17-Cl-nat
42-Mo-nat	73-Ta-181	15-P-31
19-K-nat	63-Eu-151	11-Na-23
73-Ta-nat	79-Au-197	19-K-nat
31-Ga-nat	12-Mg-nat	42-Mo-nat
	19-K-nat	73-Ta-181
	67-Ho-165	74-W-182
	74-W-186	74-W-183
	74-W-184	74-W-184
	74-W-183	74-W-186
	31-Ga-nat	41-Nb-93
		22-Ti-nat
		63-Eu-151
		56-Ba-138

BENCHMARK TESTING

- We have analyzed many CSEWG benchmarks:
  - Los Alamos fast criticals (JEZEBEL, GODIVA, FLATOP, BIGTEN, etc.)
  - ANL ZPR assemblies (6/7, 6/6a)
  - Some of the aqueous thermal criticals (ORNL1, ORNL2, ORNL10, L7, L8, L9)
  - Some of the thermal lattices (TRX1, TRX2, BAPL1, BAPL2, BAPL3)
- Using cross sections produced by TRANSX
- Using the ONEDANT and TWODANT transport codes

Results for 2 LANL bare criticals and the corresponding reflected criticals computed using 80 groups and P_3/S_{16} transport. Some numbers have improved and some have gotten worse, but the consistency between uranium and plutonium results is better.

Assembly	Quantity	Experiment	C/E VI	C/E V
Godiva	k-eff	1.000±.002	.9983	.9990
	$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.1643±.0018	.971	1.038
	$\sigma_f(^{233}U)/\sigma_f(^{235}U)$	1.59±.03	1.000	.986
	$\sigma_f(^{237}Np)/\sigma_f(^{235}U)$	.8516±.012	.960	1.044
	$\sigma_f(^{239}Pu)/\sigma_f(^{235}U)$	1.4152±.014	.977	.985
Jezebel	k-eff	1.000±.002	.9989	.9982
	$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.2133±.0023	.975	.961
	$\sigma_f(^{233}U)/\sigma_f(^{235}U)$	1.578±.027	1.000	.985
	$\sigma_f(^{237}Np)/\sigma_f(^{235}U)$	.9835±.014	.970	.979
	$\sigma_f(^{239}Pu)/\sigma_f(^{235}U)$	1.4609±.013	.975	.966
Flattop-25	k-eff	1.000±.001	1.0030	1.0054
	$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.1492±.0016	.977	1.034
	$\sigma_f(^{233}U)/\sigma_f(^{235}U)$	1.608±.003	.989	.975
	$\sigma_f(^{237}Np)/\sigma_f(^{235}U)$	.7804±.010	.979	1.054
	$\sigma_f(^{239}Pu)/\sigma_f(^{235}U)$	1.3847±.012	.983	.989
Flattop-Pu	k-eff	1.000±.0014	1.0055	1.0050
	$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.1799±.0020	.984	.974
	$\sigma_f(^{237}Np)/\sigma_f(^{235}U)$	.8561±.012	.987	1.002

Results for the fast-breeder reactor mockups. These calculations used the simplified spherical homogeneous models for these assemblies together with standard corrections originally provided by ANL. Therefore, the actual numbers shouldn't be taken too seriously. However, the change from ENDF/B-V to ENDF/B-VI does suggest how the new libraries would change existing results for actual breeder-reactor calculations.

Quantity	Experiment	Correction	C/E VI	C/E V
ZPR-6/7				
k-eff	1.000	$-.0136$	1.0070	.9997
$\sigma_f(^{238}U)/\sigma_f(^{239}Pu)$	$0.02336 \pm .0005$	$\times 1.030$	1.023	1.021
$\sigma_f(^{235}U)/\sigma_f(^{239}Pu)$	$1.061 \pm .021$	$\times$ .989	1.037	1.020
$\sigma_\gamma(^{238}U)/\sigma_f(^{239}Pu)$	$0.1400 \pm .003$	$\times 1.023$	1.057	1.082
ZPR-6/6A				
k-eff	1.000	$-.0043$	1.0063	.9894
$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	$0.02411 \pm .00072$	$\times 1.016$	.968	.980
$\sigma_\gamma(^{238}U)/\sigma_f(^{235}U)$	$0.1378 \pm .0041$	$\times 1.011$	1.003	1.042

Results for dilute homogeneous uranium assemblies using group structures with 69 and 187 groups.

Assembly	Exp k	VI 187	V 187	VI 69	V 69
ORNL-1	1.00026	0.9969	1.0003	0.9984	1.0020
ORNL-2	0.99975	0.9967	1.0000	0.9982	1.0017
ORNL-10	1.00031	0.9972	1.0000	0.9979	1.0009
L7	1.0000	1.0050	1.0069	1.0015	1.0091
L8	1.0000	1.0044	1.0082		1.0134
L9	1.0000	1.0025	1.0060		1.0089

Conclusions:

- The multiplication for the large assemblies (*e.g.*, ORNL-2) is now too small.
- The bias towards excessive multiplication for small high-leakage assemblies (*e.g.*, L7) is only slightly reduced.

A new version of ^{235}U that will greatly improve these results is in preparation by CSEWG.

Results for two thermal lattice experiments:

- TRX-1 used metal rods.
- BAPL-1 used oxide rods.
- Both were water moderated.
- Simplified models were used, and the changes shown between ENDF/B-V and ENDF/B-VI are more important than the actual values quoted.

Quantity	Experiment	69 VI	187 VI	69 V	187 V
TRX-1					
k-∞		1.1789	1.1822	1.1791	1.1829
k-eff	1.000	.9869	.9892	.9881	.9903
ρ^{28}	1.320$\pm$.021	1.033	1.023	1.040	1.032
δ^{25}	0.0987$\pm$.0010	.9993	1.004	1.013	1.018
δ^{28}	0.0946$\pm$.0041	1.021	1.036	1.021	1.037
C*	.797$\pm$.008	1.003	1.000	1.007	1.003
BAPL-1					
k-∞		1.1460	1.1462	1.1475	1.1483
k-eff	1.000	.9949	.9953	.9970	.9976
ρ^{28}	1.39$\pm$.01	1.003	1.003	1.007	1.010
δ^{25}	0.084$\pm$.002	.986	.993	1.000	1.006
δ^{28}	0.078$\pm$.004	.954	.970	.952	.968

Table give C/E values.

CONCLUSIONS

After a fairly long wait, ENDF/B-VI libraries for nuclear applications are now becoming available. The new evaluations have many improvements, but performance has worsened for a few applications. Users will have to make their own judgments about whether a change to the new libraries is justified for their own work.