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Title: ENDF70: A Continuous-Energy MCNP Neutron Data Library Based On ENDF/B-VII.0 (Viewgraphs)

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ENDF70: A Continuous-Energy MCNP Neutron Data Library Based on ENDF/B-VII.0

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Introduction to ENDF70

- ENDF/B-VII.0 neutron cross sections exist for 390 isotopes and 3 elements (but Be-7 is incomplete).
- ENDF70 contains ACE-formatted data for 392 nuclides at 5 different temperatures: 293.6, 600, 900, 1200, and 2500 K.
- Consists of 11 separate files < 900 MB each (ASCII, uncompressed); compressed it is ~380 MB
- Will be released with MCNP5 1.50.
- Changes from ENDF66 are:
  - more temperatures,
  - more nuclides including metastable states, and
  - new XSDIR with modified atomic weights.
- Processing used mainly Version 248 of NJOY; checking codes verified results

Background

- After each major release of ENDF evaluated data, the Nuclear Data Team at LANL distributes ACE-formatted libraries containing the data for MCNP
- Processing of ENDF66 library resulted in writing lots of checking codes to perform quality assurance on data
- Processing of ENDF66 also resulted in lots of upgrades to NJOY; Version 248 resolves even more issues
- Changes to both the evaluations and the ACE libraries occurred in both ENDF66 and ENDF70

List of Contents in Each ENDF70 file

File	Elements	Z numbers
endf70a	H, He, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V	1 through 23
endf70b	Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge	24 through 32
endf70c	As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo	33 through 42
endf70d	Tc, Ru, Rh, Pd, Ag, Cd	43 through 48
endf70e	In, Sn, Sb, Te, I	49 through 53
endf70f	Xe, Cs, Ba, La, Ce, Pr	54 through 59
endf70g	Nd, Pm, Sm, Eu	60 through 63
endf70h	Gd, Tb, Dy, Ho, Er	64 through 68
endf70i	Lu, Hf, Ta, W, Re, Ir, Au, Hg, Pb, Bi	71 through 83
endf70j	U, Np, Pu	92 through 94
endf70k	Ra, Ac, Th, Pa, Am, Cm, Bk, Cf, Es, Fm	88 through 91 95 through 100

New Feature 1: More Temperatures

- Doppler code can provide temperature-dependent cross sections (as part of MAKXSF)
- Interpolates values for the thermal scattering and unresolved-range in probability tables and can do so more accurately with a reasonable “upper” and “lower” bound of the temperature range

Identifier	Temperature (K)
*.70c	293.6
*.71c	600
*.72c	900
*.73c	1200
*.74c	2500

New Feature 2a: New Isotopes

- Data in ENDF70 now exists for 392 nuclides
  - 173 were released in ENDF66
  - 122 were released in ENDF60
- The wide range of fission products should help users avoid the need to lump fission products together since > 90% of the mass can now be tracked with burnup

New Feature 2b: New Metastable State Nuclides

- Data now exists for 9 isomers
- Atomic mass numbers in ZAID identifiers are unrealistic

ZAIDm = isomer ZAID =
(ZAID+300)+(m*100)
ZAID = ground-state ZAID
m = excited state (i.e. 0,1,2,3…)

- Exception is ^{242}Am/ ^{242m}Am
  - ^{242m}Am has always been 95242 (more abundant)
  - ^{242}Am (ground) is now 95642

Isotope	ZAID
^{58}Co	27058
^{58m}Co	27458
^{110m}Ag	47510
^{115m}Cd	48515
^{127m}Te	52527
^{129m}Te	52529
^{148}Pm	61148
^{148m}Pm	61548
^{166m}Ho	67566
^{242}Am	95642
^{242m}Am	95242
^{244}Am	95244
^{244m}Am	95644

New Feature 3: Changes to XSDIR

- New isotopes exist in ENDF70 that were not previously present
- MCNPX generates cross sections for isotopes that are not even present in ENDF70
- The XSDIR has been modified to contain atomic weights for a large range of nuclides with all atomic weights now coming from the source:

G. AUDI, A.H. WAPSTRA, C. THIBAULT, J. BLACHOT and O. BERSILLON "Ame2003: Atomic Mass Evaluation," November 2003, <http://www.nndc.bnl.gov/amdc/web/masseval.html> (November 2007).

*Thanks to Michael Fensin for creating the new atomic weights in xsdir

Physics Enhancements Included in ENDF70

Advanced physics enhancements made to the ENDF70 MCNP libraries include:

- Unresolved resonance probability tables*;
- Delayed fission neutron spectra*;
- Tabular angular distributions (instead of equally-likely bins); and
- Detailed charged-particle production data (cross sections and spectra).

*Note that these were included in ENDF66 but often required extra post-processing that NJOY now incorporates

Method

- Processing used Version 248 of NJOY on a LINUX machine
- NJOY modules included:
  - MODER,
  - RECONR,
  - BROADR,
  - HEATR,
  - PURR,
  - THERMR (required to prevent photon production sum issues in CONSIS),
  - GASPR, and
  - ACER (both for processing and for consistency checking)
- ^{1}H was processed using the up271 patch with Version 248 to resolve deuterium production issues
- Quality assurance checking codes included:
  - CHECK0,
  - CHECK5,
  - CHECKND,
  - CHECKND_NEUT,
  - CHECK61,
  - CHECK_HEAT,
  - CHECK_ISO,
  - CHECKTHRESH,
  - CHECK_URES,
  - CHECKXS, and
  - CHECK_LOWNUM.PL.

Seven Evaluation Changes

- ^{1}H: As with ENDF66 processing, the value for the energy of the photon from radiative capture did not take into account the recoil of the nucleus and was modified to 2.2233 from 2.2246 MeV.
- ^{45}Sc: As with ENDF66 processing, the secondary distribution for photons (MF=13, MT=3) did not have a zero point at the threshold. Additionally, the evaluation had the incorrect reference frame specified for angular distributions of (n,2n), (n,n*)a, (n,n*)p, and (n,n*c). We made changes to the evaluation and re-processed.
- ^{89}Y: Negative cross sections for MT=91 from 1.7 to 4.5 MeV were modified to be the difference between MT 4 (total inelastic) and the sum of MT's 51-90 (partial inelastic) reactions.

Seven Evaluation Changes (Cont.)

- *^{96}Zr and ^{97}Mo*: NJOY's CONSIS module identified errors in several MF=6 Law=44 "r" values that were subsequently changed from 0.999999e+1 to 0.999999e+0.
- *^{242}Am (ground):* The angular distribution for fission was missing, so we inserted an isotropic MF=4, MT=18 section.
- *^{242m}Am*: The inelastic cross sections (MT 4, 51, 52, 53, and 54) contained values of zero between 50 and 65 keV, whereas values above and below were non-zero. The cross sections below 100 keV were smoothed out by the evaluator.

Changes to ACE files

- Negative probability density functions existed for ^{153}Eu.
- Exponents less than or equal to e-37 existed for seven isotopes:
  - ^{16}O,
  - ^{40}Ca,
  - ^{42}Ca,
  - ^{43}Ca,
  - ^{44}Ca,
  - ^{46}Ca, and
  - ^{204}Pb.
- A leading non-zero threshold photon-production cross section value was found for ^{10}B.
- The ACE libraries for these isotopes were modified to correct these problems.

“Outstanding Issues”

- Problems exist with heating cross sections for 30 isotopes, including:
  - Partials adding up to more than the total, and
  - Negative results.
- Probability tables do not always sum up to the totals predicted (within 5%) and/or there are negative heating factors for 32 isotopes. Processing occurred without PURR and probability tables for these 32 isotopes.
- Opportunities for future improvements in accuracy have been identified, solutions for which probably require fundamental evaluation changes.

Opportunities for Improved Evaluations

- *Fission spectrum interpolation*: With 1 MeV intervals above 10 MeV and linear-linear interpolation, the deviations between the data and the realistic exponential shape get quite large (up to 9%).
- *Incident-energy interpolation on Major Actinides:* MCNP changes linear interpolation on incident energy in the MF6 section to some kind of unit base interpolation to smooth out the shapes. ENDF/B-VII evaluations should be changed to reflect an explicit interpolation law or MCNP should be modified.
- *Histograms for continuum distributions:* Most of the actinides, and many of the other materials based on model calculations, describe outgoing spectra in MF6 using histogram bins based on delta E. The bins should be based on sqrt(E') to minimize edges in the computed flux.
- *Delayed Neutron Spectra:* The delayed neutron spectra also use histograms with a low break at 10 keV, NJOY and/or the MF5/MT455 section of the evaluations could be modified to give high delayed neutron sources in the low energy region.
- *U-233*: There was an error in the exponent for the delayed- neutron yields for U-233 above 9 MeV, which should be e-3 instead of e-2.

Conclusions

- ENDF70 offers a wider range of nuclides and temperatures than previously available
- Use of ENDF/B-VII.0 data should improve results over ENDF/B-VI
- Followed same quality assurance process as ENDF66
- Available with MCNP5 1.50 along with ENDF70PROT, which contains processed ENDF/B-VII.0 proton evaluations