Additional Problems in Processing FENDL-3 Data for Application Libraries

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General

C-13, O-18, P-31, S-34, S-36, La-138, La-139 replaced by TENDL-2014; due to erroneous photon production data NJOY2012 got caught in an infinite loop.

If patches by Bob MacFarlane to process angular distributions from resonance parameters are included in NJOY2012, processing of Sn-116 and Sn-117 crashes with "segmentation fault" in ACER, although the source files were not changed. Evaluations that use the Breit-Wigner resonance representation are affected.

The patch to bypass the reduction of the Doppler-broadening range may result in very high limits for evaluations that have no resonance parameters, depending on the value of EH in the file. The RECONR module sets the limit to 20 MeV, regardless of the value in the source file. For such cases a new patch was prepared that sets the limit to 1 MeV if the EH value is greater than 6 MeV. The problem is that the Doppler-broadening algorithm in BROADR is unstable above 1 MeV when operating on the total cross section. This patch works satisfactorily in most cases. The ACE files are not affected because the total is defined as the sum of the partials, but differences are seen in the MATXS files.

PREPRO Doppler-broadens all cross sections up to 10 MeV, while NJOY performs Doppler-broadening only up to the upper end of the resolved resonance range (i.e the value of EH in the pointwise file). There are cases where resonance structure is given in tabular form above the resonance range. Usually such structure is obtained from data measured at room temperature and as such do not need to be Doppler-broadened. The NJOY treatment of the resonances above the resolved resonance range seems appropriate. No action is needed.

There seem to be differences in the weighting function around 12 MeV in the PREPRO sequence, which is used for validation. The differences in the weighting function give rise to differences in all multigroup cross sections. These differences should be ignored.

C-13

There is considerable inconsistency in the redundant cross sections (total and inelastic) of up to 36 %. The resolved resonance range goes up to 6.9 MeV. The existing algorithm (upnea139_up50_njoy2012) reduces the Doppler-broadening range to 1 MeV. The evaluation also

includes many very exotic reactions. No obvious inconsistencies were noted, but the multigroup libraries in particular should be checked for completeness.

N-15

Thermal capture after Doppler-broadening by BROADR is 36% higher than the one broadened by PREPRO.

F-19

The total cross section in the MATXS file differs from PREPRO by more than 40 % in the 100 keV energy range! The total cross section in the file is consistent with the sum of the partials, so this is a processing problem, probably in the Doppler-broadening of the total cross section.

Na-23

The first discrete level has resonance structure. No Doppler-broadening is applied in NJOY, which is probably correct.

Si-29

The discrete inelastic cross sections have a discontinuity at around 8 MeV, but this is a problem in the source evaluated data that should be looked at; it is not a processing problem. The discontinuity is observed when plotting the cross sections on a linear scale. A similar discontinuity also appears in the (n,alpha) channel.

P-31

The P-31 evaluation replaced by TENDL-2014 contains many exotic reactions explicitly. Data processing went through without problems, testing of the files in application codes was not conducted yet.

S-32

A small difference in the Doppler-broadened total and alpha-emission cross sections below 0.05 eV retrieved from the ACE file compared to PREPRO results is observed. The difference is small and originates from the differences in the Doppler-broadening assumptions of the discrete level alpha emission between NJOY and PREPRO (the former skips Doppler-broadening of this reaction).

S-33

A similar problem as for S-32 is observed for the alpha and the proton emission channels at thermal energies.

S-36

The capture cross section in the unresolved resonance region does not seem to have the right shape. This is a problem with the evaluated data file and not a data processing problem.

K-39

The shape of the capture cross section in the source evaluated data file is very strange and should be looked at. This is a problem with the evaluated data file and not a data processing problem.

K-40

The evaluated data file contains a ladder of uniformly-spaced resonances. Particle-emission reactions are represented by straight lines in log-log scale, giving rise to differences due to Doppler-broadening assumptions at thermal energies.

K-41

The same comment applies as for K-39.

Sc-45

The total cross section in the source evaluated data file is inconsistent with the partials by up to 4 %. This leads to an inconsistency in the processed MATXS library.

Fe-56

The alpha-emission cross sections for the last two discrete levels from the MATXS library seem to be corrupted. It is (yet) uncertain if the error is in the file or just in the retrieval code.

Fe-57

The total cross section retrieved from the MATXS file is 31 % lower than the equivalent processed with PREPRO. The inconsistency is not in the basic file, but seems to appear after Doppler-broadening.

Zr-90

When assembling ACE and MATXS files, NJOY reconstruct gas-production cross sections from the contents in MF6/MT5, while PREPRO plots only what is originally in the file. The contents of the ACE and MATXS files are correct.

Lu-175

There is a big difference of a factor of ten due to the Doppler-broadening approach of the alpha-emission cross section at thermal energies.

Lu-176

The same problem as in Lu-175 is observed. The difference amounts to about a factor of two, but the cross section is significant.

W-180

Some discrete-level alpha-emission cross sections have spurious spikes at low energies.

Re-185

There is a big difference of a factor of fifteen due to the Doppler-broadening approach of the alpha-emission cross section at thermal energies.

Re-187

There is a big difference of a factor of fifteen due to the Doppler-broadening approach of the alpha-emission cross section at thermal energies.

Pt-190

There is a big difference of a factor of seven due to the Doppler-broadening approach of the alpha-emission cross section at thermal.

Pt-192

There is a big difference of a factor of five due to the Doppler-broadening approach of the alpha-emission cross section at thermal.

Pt-194

There is a big difference of a factor of five due to the Doppler-broadening approach of the alpha-emission cross section at thermal.

Pt-195

There is a big difference of a factor of 1.6 due to the Doppler-broadening approach of the alpha-emission cross section at thermal.

Pt-196

There is a big difference of a factor of fifteen due to the Doppler-broadening approach of the alpha-emission cross section at thermal.

Pb-206

There seems to be a problem with the discrete level proton-emission cross sections, as well as with the discrete level alpha-emission cross sections. It could be a problem with data retrieval from the MATXS file.