ENERGY BALANCE OF ENDF/B-VI

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ABSTRACT

ENDF/B-VI through Release 2 has been tested for neutron-photon energy balance using the HEATR module of the NJOY nuclear data processing system. The situation is much improved over ENDF/B-V, but there are still a number of materials that show problems.

I. INTRODUCTION

Nature always tries to conserve energy, and she always succeeds. Nuclear data evaluators don't always do so well. A previous study[1] showed that many of the evaluations of ENDF/B-V contained neutron and photon distributions with average energies that were not consistent with the energy available for the reactions. A similar study has now been carried out for ENDF/B-VI through Release 2 (June 1993) using capabilities included in the HEATR module of the NJOY nuclear data processing system.[2]

Nuclear heating arises from the energy of the charged products of a nuclear reaction, including the recoil nucleus. This energy is deposited close to the site of the reaction, but the emitted neutrons and photons travel to other parts of the system and deposit their energy by further reactions. Previous to the ENDF-6 format,[3] it was not possible to give explicit distributions for the charged reaction products. Therefore, we were forced to compute the heating factors (which are also called KERMA factors, for kinetic energy release in materials) by subtracting the energy of the emitted neutrons and photons from the available energy (the energy-balance method). Sometimes, due to errors, approximations used, or limitations in the formats, evaluators would put too much energy into a photon distribution. This would result in a negative value for the heating, which would naturally cause concern to the users. However, it should be noted that this negative value would just compensate the excess heating caused by the erroneous photon distribution in a system large enough so that the photons could not escape. We have been using the energy-balance KERMA factors for years now, with confidence that they will be sufficient for large systems, and with fear that they will lead to bad results for small systems.

For simple reactions, such as elastic scattering or (n,n$'$) to a discrete level, it is possible to compute the recoil energy by kinematics. For other reactions, it is possible to calculate crude kinematic limits for the total charged-particle energy. These limits can also be reinterpreted to give minimum and maximum values for the photon energy production. These kinds of kinematic limits give a much better picture of how well an evaluation satisfies energy conservation than a simple search for negative KERMA values. The HEATR module of NJOY has a kinematic testing option intended for use by evaluators. This option causes detailed information to be printed out on the average energies of reaction products *vs* incident energy, on how well the heating numbers agree with their kinematic limits, and one how well the total photon energy production agrees with its kinematic limits. Graphs comparing the heating or photon production to the kinematic limits can also be prepared.

Some of the new evaluations prepared for ENDF/B-VI take advantage of new features in the format[3] that allow charged-particle and recoil distributions to be given explicitly. For these cases, the heating can be computed directly, and there is no possibility of negative KERMA factors. These modern evaluations also locate the photon emission data in the same section with the neutron and charged-particle emission data. Therefore, energy conservation can be checked reaction by reaction without having to rely on HEATR. As will be discussed below, we recommend that this approach be used for future evaluations.

II. RESULTS

The NJOY option for kinematic testing has been used to analyze all the materials of ENDF/B-VI (including corrections through Release 2 of June 1993) that have photon production data given. The materials that pass the tests within acceptable accuracy for all neutron energies are listed in Table 1. The materials that give explicit charged-particle distributions in ENDF-6 format are F, Cr, Mn, Fe, Ni, Cu, and Pb.

Table 1. ENDF/B-VI Materials With Good Energy Balance

Material	Material
^{1,2}H	^{nat}V
^{6,7}Li	^{50,52,53,54}Cr
^{9}Be	^{55}Mn
^{10,11}B	^{54,56,57,58}Fe
^{nat}C	^{59}Co
^{14,15}N	^{58,60,61,62,64}Ni
^{16}O	^{63,65}Cu
^{19}F	^{206,207,208}Pb
^{nat}Ca	

Note that many of the most important structural materials are on this list. Figure 1 shows the improvement obtained between ENDF/B-V and ENDF/B-VI for chromium. Similar improvements were obtained for ^{55}Mn and nickel.

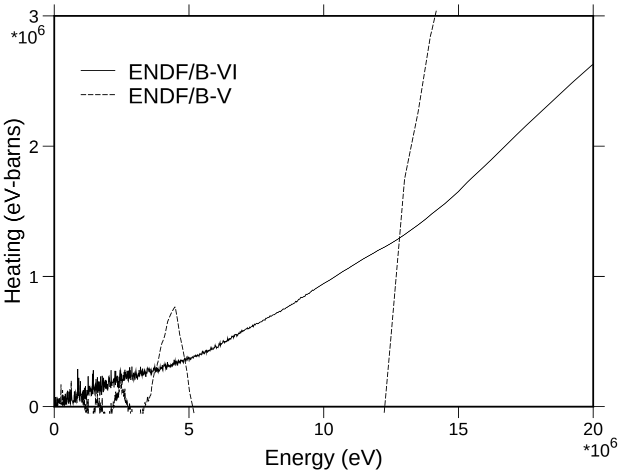

Figure 1. KERMA comparison for chromium.

The rest of the materials have been classified as "good," "fair," or "poor" over three energy ranges: thermal, fission (basically .1 to 2 MeV), and fusion (basically 2 to 14 MeV). Materials that rate as having "poor" energy balance have negative heating values, have values less than half the minimum kinematic limit, or have values more than twice the maximum limit. Materials rated as fair lie between those rated as good and those rated as poor. Table 2 shows these classifications for all the materials not listed in Table 1.

Table 2. Classification of ENDF/B-VI Materials with Energy-Balance Problems by Energy Region

Material	Thermal	Fission	Fusion
^{23}Na	good	good	poor
^{nat}Mg	good	fair	fair
^{nat}Si	good	good	fair
^{31}P	good	good	poor
^{32}S	good	good	fair
^{nat}S	good	fair	fair
^{17}Cl	poor	fair	poor
^{nat}K	poor	poor	poor
^{45}Sc	good	fair	good
^{nat}Ti	good	fair	poor
^{nat}Ga	fair	poor	fair
^{89}Y	good	fair	fair
^{93}Nb	good	fair	poor
^{nat}Mo	poor	poor	poor
^{nat}In	good	fair	fair
^{138}Ba	fair	fair	fair
^{151}Eu	good	poor	poor
^{153}Eu	good	fair	fair
^{165}Ho	good	poor	fair
^{181}Ta	fair	poor	poor
^{182}W	good	fair	poor
^{184}W	good	poor	poor
^{182}W	good	poor	poor
^{182}W	good	poor	fair
^{197}Au	good	poor	fair
^{209}Bi	good	good	poor

Energy-balance problems for the heavier isotopes are not always serious, because the KERMA factors are small with respect to gamma heating. The thermal problems can normally be fixed with a simple Q value change. Some of the other materials could be improved with patches, but we believe that it would be better to do a proper reevaluation using modern methods. Most of the materials with problems were carried over from ENDF/B-V (or earlier versions) and are due for review.

III. ADVICE FOR EVALUATORS

Analysis of the source of the energy-balance problems in the materials of ENDF/B-VI reveals which methods work well and which tend to cause problems. By stating these results as "advice to evaluators," we hope to contribute to improved evaluations for ENDF/B-VI, and also to help evaluators for other evaluated data systems that make use of ENDF formats, such as JEF in Europe, BROND in Russia, and JENDL in Japan.

Suggestion 1: Do isotopic evaluations. It is impossible to compute the available energy of a reaction in an element without resorting to unsatisfactory methods, such as giving an energy-dependent Q value to HEATR.

Suggestion 2: Give discrete photons for levels. Many of the energy-balance problems in the fission-reactor energy range are due to giving total inelastic or nonelastic photon production sections (MT=3 or 4) using a coarse energy grid that is not consistent with the reaction cross sections for inelastic scattering given by levels (MT=51, 52, etc.). A typical consequence of this might be seen for a photon production bin that runs from 1 to 1.5 MeV for a material having a level with a threshold at 1.2 MeV. Photons from that level will be seen between 1 and 1.2 MeV, leading to a negative spike in the energy-balance heating. One solution is to continue using MT=3 or 4, but change to a very fine incident-energy grid. A better one is to give photon yields or transition probability arrays for all the discrete photons from the levels in MT=51, 52, etc. The resulting production cross sections will track the neutron cross sections precisely, and it is easy to check the energy balance for each level. The use of photon yields rather than production cross sections also handles cases where the inelastic cross section shows resonance features, such as ^{nat}Mg.

Suggestion 3: Use File 6 for continuum reactions. The new File 6 capabilities introduced for the ENDF-6 format allow the evaluator to give explicit distributions for all the particles emitted from a reaction, including the recoil nucleus. Putting the photon emission in the same section that describes the neutron, charged-particle, and residual nucleus emission makes it very easy to check for energy conservation reaction by reaction. If the recoil spectrum (or average energy) is not provided, the processing code has to attempt to reconstruct it by energy balance or by kinematics. But the processing code doesn't have all the information that was available to the evaluator from the model code, such as the correlation between the energies of first and second neutrons in an (n,2n) reaction. Therefore, it has to make crude assumptions. It is much better to put this burden on the evaluator.

Suggestion 4: Be careful with interpolation. When it is not possible to follow suggestions 2 and 3, pay careful attention to the energy grid used for photon production in sections with MT=3, 4, 91, etc. These grids are almost always too coarse in existing evaluations, thus leading to predictions for photon emission at energies between the grid points that are not consistent with the energetics of neutron emission. Adding a few extra photon production yield points with the corresponding spectra can dramatically improve the energy-balance results.

Suggestion 5: Use as many partial reactions as possible for photon production. There have been cases where an evaluation used a simple total nonelastic photon production reaction (MT=3) adjusted to fit experimental data. If this nonelastic cross section is broken up into separate parts (*e.g.,* MT51, MT52,... MT91, MT16, MT107), the chances are better that problems in the photon production data will be detected by ridiculous yields, unreasonable shapes, or bad energy balance. The best results are usually obtained when nuclear models are used to fit the photon production data. In such cases, the partial photon production reactions are normally available from the model, and it is a shame to throw the results away. Put all the partial reactions from the model into the evaluation.

Following these suggestions makes the evaluation process more difficult and it makes the resulting files larger. The suggestions clearly are aimed towards evaluators who make extensive use of nuclear models to fill in the parts of the data sets that are not well covered by experimental data. However, the increased range of applications of modern nuclear data make it necessary to hold ourselves to higher standards. Evaluations that were sufficient for fission reactor analysis may not be adequate for fusion reactors, medical applications, accelerator transmutation projects, and so on.

IV. CONCLUSIONS

The energy balance of ENDF/B-VI is much improved over ENDF/B-V, especially for the important structural materials that appear in large concentrations in nuclear systems. This implies that nuclear heating and radiation damage predictions will be more reliable using the new data. However, there are still materials with significant energy-balance problems. They should be reexamined using modern methods.

REFERENCES

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