ENERGY BALANCE OF ENDF/B-VI

Robert E. MacFarlane
Nuclear Theory and Applications
Los Alamos National Laboratory

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INTRODUCTION

- Nature always tries to conserve energy, and she always succeeds.
- Nuclear data evaluators don't always do so well!
- A study in 1979 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 new study has now been carried out for ENDF/B-VI through Release 2 (June 1993) using the HEATR module of the NJOY nuclear data processing system.

NUCLEAR HEATING (KERMA)

- 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.
- 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, it was not possible to give explicit distributions for the charged reaction products.
- Energy Balance Method: heating = available energy − neutron energy − photon energy

ENERGY-BALANCE ERRORS

- The energy-balance KERMA is a sensitive indicator of energy conservation problems in an evaluation.
- Example: evaluator puts too much energy into the photon production term.
- This will make the energy-balance heating negative and upset users.
- But this negative value will just compensate the excess heating caused by the erroneous photon production in a large system.
- 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.

KINEMATIC CHECKS

- For simple reactions, it is possible to compute the recoil energy by kinematics.
  - elastic scattering
  - (n,n′) to a discrete level
- 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.
- Kinematic testing option of HEATR in NJOY:
  - Mostly intended for evaluators.
  - Prints average energies of reaction products *vs* incident energy.
  - Checks the heating numbers against their kinematic limits
  - Checks the total photon energy production against its kinematic limits.
  - Prepares graphs comparing the heating or photon production to the kinematic limits.

NEW FILE 6 EVALUATIONS

- Some new evaluations use new features in the ENDF-6 format to give explicit charged-particle and recoil distributions.
- The heating can be computed directly.
- There is no possibility of negative KERMA factors.
- Photon emission data is located in the same section with the neutron and charged-particle emission data.
- Energy conservation can be checked reaction by reaction without having to rely on HEATR.
- We recommend that this approach be used for future evaluations.

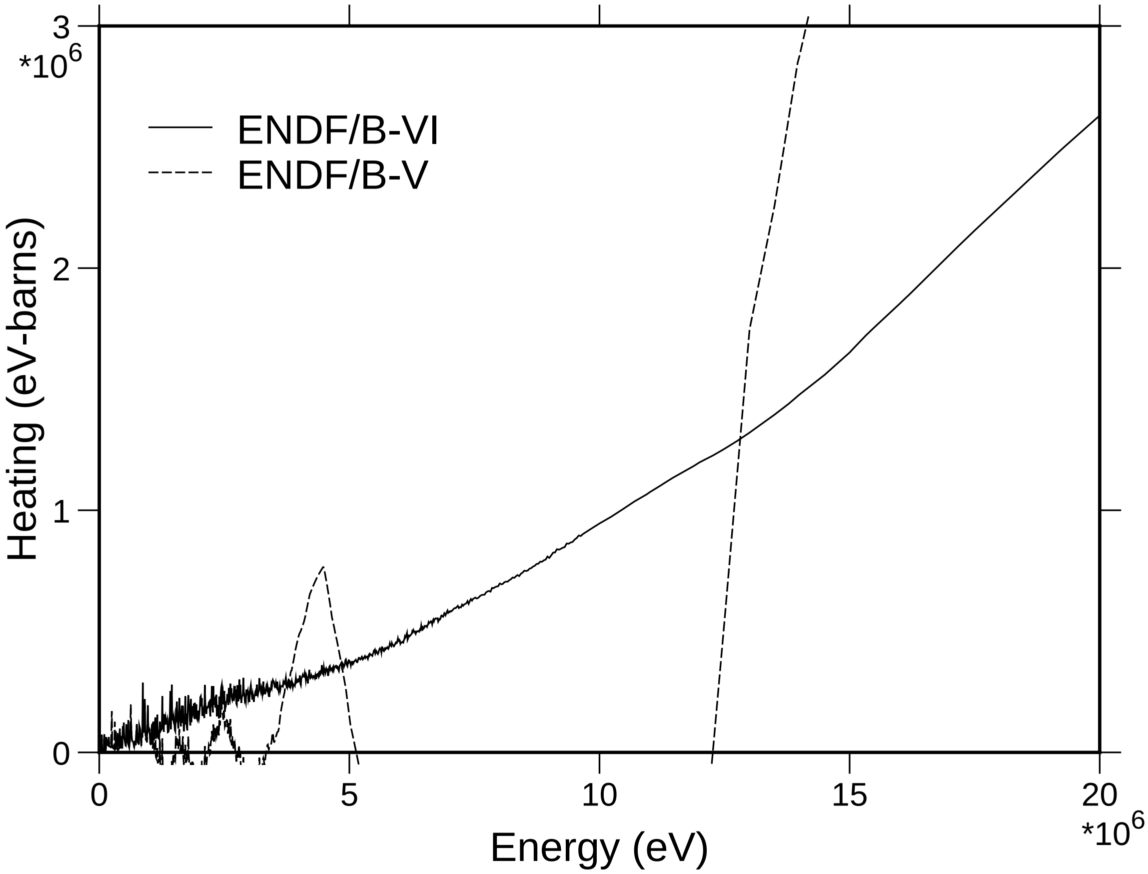
RESULTS

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.

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	

Materials using File 6: F, Cr, Mn, Fe, Ni, Cu, and Pb.



KERMA comparison for chromium.

PROBLEM CLASSIFICATION

- By energy range:
  - **Thermal**: .0253 eV
  - **Fission**: .1 to 2 MeV
  - **Fusion**: 2 to 14 MeV
- By severity of the problems:
  - **Good**: no important problems.
  - **Fair**: no negative KERMAs, most deviations less than twice the upper kinematic limit and greater than half the lower kinematic limit.
  - **Poor**: negative KERMA values, frequent deviations above twice the uppper kinematic limit or below half the lower limit.

MATERIALS WITH PROBLEMS

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

OBSERVATIONS

- Energy-balance problems for the heavier isotopes are not always very 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 proper reevaluations using modern methods.
- Most of the materials with problems were carried over from ENDF/B-V (or earlier versions) and are due for a review.

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 other evaluated data systems that make use of ENDF formats, such as JEF in Europe, BROND in Russia, and JENDL in Japan.

ADVICE, CONTINUED

- Suggestion 1: Do isotopic evaluations.
  - It is impossible to compute the available energy of a reaction in an element.
  - Avoids the use of energy-dependent Q values in HEATR.

ADVICE, CONTINUED

- 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.).
  - This leads to positive and negative spikes in the energy-balance KERMA.
  - One solution is to continue using MT=3 or 4, but change to a very fine incident-energy grid.
  - A better solution 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.
    - It is easy to check the energy balance for each level.
    - It also handles cases where the inelastic cross section shows resonance features, such as ^{nat}Mg.

ADVICE, CONTINUED

- Suggestion 3: Use File 6 for continuum reactions.
  - File 6 allows 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.
  - But the processing code doesn't have all the information that was available to the evaluator from the model code.
  - It is much better to put this burden on the evaluator.

ADVICE, CONTINUED

- 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.
    * This leads problems for photon emission at energies between the grid points.
    * Adding a few extra photon production yield points with the corresponding spectra can dramatically improve the energy-balance results.

ADVICE, CONTINUED

- 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.
    - The partial photon production reactions are normally available from the model.
    - It is a shame to throw the results away.
    - Put all the partial reactions from the model into the evaluation.

CONSEQUENCES OF THE SUGGESTIONS

- The evaluation process becomes more difficult.
- The evaluated data files become larger.
- But these higher standards will be needed to handle the increased range of applications of modern nuclear data.
  - fusion reactors,
  - medical applications,
  - accelerator transmutation projects,
  - etc.

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.