Cross Section Evaluation Working Group

Minutes of the Meeting on Validation of the ENDF/B-VII beta2 Library

Held on June 27, 2006 at Brookhaven National Laboratory

Minutes prepared by P. Oblozinsky, NNDC and M.B. Chadwick, LANL
July 7, 2006
www.nndc.bnl.gov/meetings/valid2006/

Participants

24 participants attended the meeting, including 22 participants from 8 US laboratories, 1 from Europe and 1 from Russia, see table at the bottom of the present document.

Conclusions

1. Reported results on validation of ENDF/B-VII beta2 are very encouraging. Despite of this, in view of considerable number of changes compared to b1 (120 updated materials in the neutron sublibrary alone) and desire to fix some of the remaining deficiencies, the meeting decided to postpone VII.0 release for several months.

2. ENDF/B-VII beta3 testing version should be issued. The schedule is as follows:
   - Release of b3 in Sep 15, 2006 with the understanding that b3 = VII.0,
   - Validation of b3 in the next 6-8 weeks, and
   - Review of b3 at the CSEWG Annual Meeting in November 6-8, 2006 and official release of VII.0 shortly afterwards.

3. Special issue of Nuclear Data Sheets on the ENDF/B-VII.0 library should appear simultaneously with the release of the library. The issue should contain a summary paper (~100 pages) describing the whole library, along with several more detailed papers devoted to neutron sublibrary. These latter papers should be devoted to neutron reaction evaluations (U isotopes by LANL, resonances by ORNL, evaluation methodology by BNL, Gd by BNL), processing (LANL) and benchmarking (Petten).

Action Items (based on notes taken by Mark Chadwick)

This summary to-do-list complements Mike Herman's list, he has a long list of items that have already been identified and fixed.

LANL:

1. Np resolved resonance (RR) issue, noted by Brown
2. MacFarlane has noted KERMA deficiencies for many evaluations. This is a typical case, as it is hard to represent all the secondary particle and gamma ray

spectra sufficiently accurately. Herman will study this in case it reflects an EMPIRE problem.

3. MacFarlane will fix NJOY
    a. Patch that would allow to use interpolation law 22 in MF=5.
    b. ACER patch (multiplicity flag) for TYR needed for 232Th, Pa231,233
    c. ERRORR patch for processing 232Th covariances above the resonance range. (The first problem may not be a problem for criticality but probably does for fixed source simulations).
4. Check 191,193Ir evaluations completed by BNL (based on LANL dosimetry x/s).
5. p+13C has a problem, evaluation is incomplete (Page, Hale)
6. Add uncertainties on C/E for all criticality plots (Skip)
7. HEU-MET-FAST poly slab results look slightly high (0.2-0.3), but vdMarck's results appear closer to 1. Why?
8. Pu-SOL-THERM. ENDF6 and 7 very similar – smallish bias above 1 (0.3-0.5% say) and there's quite a range
9. Be reflector bias… many comparisons look better for Pu-HEU-Be etc configurations (MIX-MET-FAST-007). But we have now looked at some new experiments (-066 and -077 experiments from LLNL) – but these have come down ~0.5% too low.
10. Pb reflector improvements often look very good for fast systems. LCT10 looks high. There is a fast case HMF57 where we may have differences with SVM – we see a big bias for one experiment (2% high) – that got better than the previous 4%. Should see if we can locate a Sublet MCNP deck for Valduc Pb reflector.
11. HEU/D2O. Similar to B-VI. Bias with increasing D fraction. (Fast leakage matters here, according to Russ). But VI.4 looks better with old D distributions in fast region. (Bob wonders if there are some thermal scattering kernel issues here)
12. Get Heinrichs to recalculate 233U data for us? Just to confirm our results?
13. Russ Mosteller: Zeus HEU-Graphite 4 cases. Big swing from Zeus1-4 = almost 1% - an energy dependent bias. Russ wonders if this is a probability table issue. The bias was always there with early evaluations. U235 in the unresolved range. Luiz wonders if the SLBW is insufficiently accurate in the unresolved range & impacts self-shielding aspect of the calculation. Russ thinks Cu makes no difference – though Bob M had some success in looking at this as Cu has 50% absorption in the problem (but he had less success with the ones involving graphite).
14. Russ: Other ZEUS benchmarks suggest Cu is an issue, and Russ recommends looking at fast range. (He got better results with the B-V data).
15. Russ: Pu-nitrate solutions. Similar to B-VI. Thermal 239Pu should be reviewed. PNL MOX lattices do a good job with beta2 – better than before.
16. Russ: D2O. Reflected spheres got worse since 6.4 – due to more forward-peaked ang dist from Hale and so more leakage. (But unreflected cylinders got better – Russ thinks these unreflected cylinders are incompatible with the sphere expts – and Russ trusts the sphere ones more), Russ and Bob need to talk offline, since Bob referred to a plot of Skip's on the D/U ratio that suggests the 2 classes of experiment (004 v 020) may be more consistent. (Mike noted that Townsend recommends a new measurement for n+D).

Steven van der Marck, NRG Petten:

17. 242,242mAm crashes in HEATR. Pa231, 233 andTh232 – wrong TYR from NJOY. Es-253 incomplete. Rh-103 – MCNP expung error –could it be that the file is too big somewhere. (M. Duijvestijn noted Am problems).
18. Used MJOY-99.125 and MCNP-4C3: 723 ICSBEP benchmarks! Uses lower statistics than Bob & Skip generally.
19. LCT6 v good. New LCT& Valduc results very good. Pitch removed.
20. Intermediate IEU-COM-INTER look v good (Bigten ZPR, Jemima etc, except one not great – ZPR involving tungsten.
21. Difference between LANL and vdMarck for HMI01. Steel involved. Bob could have used a different input deck.
22. ZEUS shows a trend (similar to earlier versions). Russ thinks it is the probability tables in the unresolved resonance treatment. MacFarlane studied the copper and could not fix this problem based on copper changes.
23. Be changes in HMF5. Lower but not noticeably worse.
24. Pu fast. PMI02 5% high – Dick says everyone gets this wrong.
25. Pu solutions. Scattered results. Averaged k-eff… Pu looks high.
26. Lead LCT10. Thermal biases still high (steel, uranium look good as reflectors in the thermal region). In fast range – lead and Al reflectors look better. But HMF64, 57 these lead reflected fast benchmarks look bad. Differences between Skip and vdMarck noted for HMF057.
27. Gd: MHF10 look good; ICT looks good for Gd and Cd. BUT: LCT5. Beta2 is slightly high. Some look poor – though overall not really worse. (Russ might be able to recalculate some B&W benchmarks.) It is a soluble material for reprocessing – and this valuable, PROFIL mass spec experiments to test capture - C/E testing for Gd? Dick McKnight thinks the US have these data – would be great to simulate these.
28. Fluorine HST-39 shows a problem.
29. Tungsten – all show a high bias (in HMF60,67, PMF5, etc)
30. vdMarck versus Skip HEU-MET: differences for polyethylene – vdMarck calculates close to 1, need to resolve.
31. Pulsed sphere benchmarks, LLNL. Mg looks bad.
32. NIST water spheres – reaction rates. Interesting…. But how useful???
33. B-eff. Calc using his own method, for reference calculations for fast & thermal systems. Fast range – look fine. In thermal case, beta-2 looks a bit high (5%) – JENDL3.3 looks better, and SVM thinks they were adjusted. Cecil says that a reduced delayed thermal nubar (that we plan to make) will fix this. SVM would like someone to verify his method (using a non Monte Carlo approach), and advises caution in believing his results!

Other laboratories:

34. McKnight – Re verification: McKnight has good agreement with VIM code too – could be added into paper. (Also cross checks on processed data going on – Bob and Bob sent ANL the processed data).

35. ZPR. When just 238, thing looks v good for beta-2. ZPR9 assemblies show problems with tungsten reflectors. The u9 core is like Bigten – and looks v good. Other exotic materials (Nb? Be?) for space nuclear applications show questions, but Dick notes that the benchmark specifications are questionable.
36. Trumbull & Lubitz, KAPL: O16 has 32% reduction in n,a from 2.4-8.9 MeV. KAPL supports n,a 16O change; neutral re Bob's H kermel change – some improvements, some a wash.
37. Trumbull & Lubitz (KAPL): Zr
    a. Perturbations studied - SG23 led to a reduced reactivity. 5% changes in disappearance, scattering, P1 moment. Reactivity most sensitive to scattering in 90Zr (not capture!). Looked at sensitivities in different regions. Sees a case, based on integral studies on some thermal assemblies, that elastic scattering should/could be increased – especially in fast region >400 keV. Suggesting making no changes to the resonance range – resolved or unresolved. But what about changing the high-energy elastic scattering? Recommends nothing for B-VII. However, plausibly Zr90 elastic could be studied (& increased >0.4 MeV).
    b. MacFarlane noted that some of our 233U testing depends on Zr too – changes might impact the 233U testing, so be aware of this. "SG23 over-absorbs in propriety benchmarks at KAPL & so will not use it"!). Russ says look at SB2.5 since true critical and didn't have a blanket around it, and it also had some Zr in.
    c. Conclusion on Zr – could have a study to look at 90Zr with 5% higher elastic > 0.4 MeV – but be careful about how this impacts 233U testing. (Note that they didn't preserve the total in the sensitivity studies. This might complicate things, since presumably we wouldn't have much freedom to change the total cross section).
38. Zerkle (Bettis). Accept the O16 and the kernel changes. The impacts on the trends tend to cancel each other, giving good results.
39. Zerkle (Bettis). Looked at some decay file checking, did some consistency checks, with an eye to impact on decay heat analyses, feedback given to BNL, to be fixed by Sonzogni.
40. File 1/458. Energy release in fission. 18 element LIST records. Gives constants (at thermal) – including EFR – k.e. of the fragments. Could expand the definition of the LIST record to represent polynomials instead - so have the data in the ENDF file itself. ORNL didn't think this
41. Pronyaev has shown ratio of beta2/Atlas for thermal capture x/s.
    a. Some discrepancies noted for 208Pb, 232Pa. Pb208 is a factor of 2 off. Will this impact Pb data testing?
    b. For capture resonance integral… 232U looks very low.
    c. Let's check Pu240 too to make sure it's OK (Dick) as this is important for reactor calculations.
    d. Pavel will distribute the list of the most important problems.
42. Standards/Pronyaev
    a. Standards used in beta2, except for 10B nn' and n,tot. (Nobody saw this really as a problem – this inconsistency between standards and beta2). He

noted that most covariances are not included in beta2. MBC didn't see this as a problem since they can be gotten from the sublibrary. We don't have n+H covariances anywhere – should Gerry try to generate these – is it feasible, or necessary.

b. Pronyaev noted the lower 233U standards value for nubar. We should adopt this.
c. 235U nn' at thermal is higher (15.08 14.something) – we should note in the "future work" section. There was a precise measurement of the scattering length from interferometry for 235U.
d. 239Pu capture n,g higher (271.5 v 270.33) in Standards – we could try adopting this to see if it helps thermal Pu solutions! But Pronyaev plotted Pu solutions versus Pu enrichment and noticed that for high enrichment 239Pu the extra reactivity moves to zero-ish – so maybe 239Pu is OK – so maybe it's due to other Pu isotopes (eg 240Pu?).

43. Covariances
    a. Dick McKnight would be really keen to get 235,8U (and 239Pu covariance data). Will 235,8U really be ready? ORNL's 235 is done, 238U is in progress.
    b. Dunn – would like 235U covariances. LANL is doing this FY – might make it in time for B-VII?
    c. Summary – we will take what we can, but can't promise this. 235U is the most likely – Don Smith would give a review.
44. BNL prepared RR list that could be improved. Of these, people thought Eu155 possibly important (source for Gd), as well as Nd155, 156.
45. Processing (see also action item #3)
    a. MacFarlane - 99.125 version processes most things pretty well. We have a few updates. We have run through many compilers with & without optimizations – this has helped solve bugs.
    b. Law22 interpolation is in progress. Bob hasn't tried everything – some FP should be fixed. Needs to look at TYR.
    c. BNL needs an official version of NJOY by late August.
    d. BNL needs latest version of ERRORJ. By August ORNL will make PUFF available, and will make ERRORJ available. We want an official version that can be used on B-VII. Herman asks if ERRORJ can be put on web.

<u>Meetings of interest</u>

- Special session for Boston ANS meeting will be finalized in 2 weeks.
- There will be Washington ANS meeting at the end of November 2007.
- There will be PHYSOR 2007 and 2008.

Detailed Action Item List for LANL (based on notes taken by Mark Chadwick)

Phil Young

- Steven vdMarck says: 242,242mAm crashes in HEATR. Help resolve this – Bob MacFarlane didn't seem to have a problem (for Talou, MacFarlane, Kawano, Young)

- Using the lower 233U nubar thermal standard was blessed. Send Mike at BNL gets the revised file.
- Pronyaev has shown ratio of beta2/atlas for thermal capture x/s. Some discrepancies were noted for 208Pb, 232Pa. Pb208 is a factor of 2 off. Will this impact Pb thermal data testing (as capture is v small)? For capture resonance integral… 232U looks very low. Let's check Pu240 too to make sure it's OK (Dick) as this is important for reactor calculations. Pavel will distribute the list of the most important problems. (Young and Kawano)
- Steven vdMarck: B-eff. Calc using his own method, for reference calculations for fast & thermal systems. Fast range – look fine. In thermal case, beta-2 looks a bit high (say 5%) – JENDL3.3 looks better, and SVM thinks they were adjusted. Cecil says that a reduced delayed thermal 235U nubar will fix this. Phil/Toshihiko/Bill – can we discuss lowering the thermal 235U delayed nubar, a-la-JENDL – as recommended by Cecil. Cecil says that an ANS group bed by Mike Bradey is studying this, & informally says their conclusion to support the reduction is a done deal.
- FYI – NO WORK NEEDED! 235U nn' at thermal is higher (15.08 v 14.something) compared to Standards – we should note in the "future work" section. There was a precise measurement of the scattering length from interferometry for 235U.
- 239Pu capture n,g higher (271.5 v 270.33) in Standards – we could try adopting this to see if it helps thermal Pu solutions & reduce thermal criticality slightly! But Pronyaev plotted Pu solutions versus Pu enrichment and noticed that for high enrichment 239Pu the extra reactivity moves to zero-ish – so maybe 239Pu is OK – so maybe it's due to other Pu isotopes (eg 240Pu?). Open question. (Young/Kawano/Chadwick/MacFarlane)

Toshihiko Kawano

- Possible format issue in 237Np RR file, noted by Brown at Livermore
- Work with MacFarlane and Mosteller to test final 237Np file on Np-U composite assembly
- Pronyaev has shown ratio of beta2/atlas for thermal capture x/s. Some discrepancies noted for 208Pb, 232Pa. Pb208 is a factor of 2 off. Will this impact Pb thermal data testing (as capture is v small)? For capture resonance integral… 232U looks very low. Let's check Pu240 too to make sure it's OK (Dick) as this is important for reactor calculations. Pavel will distribute the list of the most important problems. (Young and Kawano)
- Give feedback to MBC and Little etc on whether completion of 235U (and maybe 238U) covariance data is feasible for send of sept, for B-VII release. (with Talou).
- Discuss with MBC KAPL's interest in changing the 90Zr SG21/B-VII elastic cross section above 400 keV, and discuss with Herman and Lubitz. (with Young, Talou, mbc). Herman would do the work!
- Steven vdMarck: B-eff. Calc using his own method, for reference calculations for fast & thermal systems. Fast range – look fine. In thermal case, beta-2 looks a bit high (say 5%) – JENDL3.3 looks better, and SVM thinks they were adjusted. Cecil says that a reduced delayed thermal 235U nubar will fix this.

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Stephanie Frankle

- For the B-VII paper: Data testing of pulsed sphere 235,8,9 LLNL data, versus 'final' B-VII files – say beta2 files, for making 3 pictures for our B-BII paper. It's possible that your earlier testing is just fine, since I don't think the relevant parts of these 3 actinide evaluations has changed recently. A few supporting paragraphs for the B-VII paper text, together with the 3 figures.

Morgan White

- For the B-VII paper: A few paragraphs on data testing of the photonuclear data, with a few figures showing the MCNP simulations v Barber and George data. Say for HEU, and for 1 or 2 other materials. Also, some text describing the (limited) DN testing we did, comparing results from 2 different spheres. (Little and White)

Russ Mosteller

- Are the industry benchmark expts for Gd testing usable?
- Repeat Np237 data testing with final beta3 file.
- Provide data testing paragraphs to Skip – especially some sentences on n+D ang dist, and intermediate energy 235U data, for the future work section,

MacFarlane

- Reaction rate results from data testing. Also, Pu and Am nf and n2n rates in Pu flattop
- NJOY. Law22 mf5 fix; ASER TYP patch. ERRORR patch for Th232 covariances;
- Steven vdMarck says: 242,242mAm crashes in HEATR. Help resolve this – Bob M didn't seem to have a problem. (for Talou, MacFarlane, Kawano, Young)
- Ask David Heinrichs at LLNL to also calc 233U assemblies, just as a check.
- Differences between Skip and VDM noted for HMF057 (lead) – track down, with Skip. (Likewise for other differences with VDM results, eg polyethylene)
- 239Pu capture n,g higher (271.5 v 270.33) in Standards – we could try adopting this to see if it helps thermal Pu solutions & reduce thermal criticality slightly! But Pronyaev plotted Pu solutions versus Pu enrichment and noticed that for high enrichment 239Pu the extra reactivity moves to zero-ish – so maybe 239Pu is OK – so maybe it's due to other Pu isotopes (eg 240Pu?). Open question. (Young/Kawano/Chadwick/MacFarlane)

Kahler

- Add uncertainty bars onto all criticality C/E plots
- Take lead on writing data testing part of B-VII paper
- Lead work to include Madland's energy release in B-VII (set up a meeting with Madland, MacFarlane, Little, Frankle, me, Young, etc to get this going & brainstorm)
- Differences between Skip and VDM noted for HMF057 (lead) – track down, with MacFarlane. (Likewise for other differences with VDM results, eg polyethylene)

Talou/Trellue

- Check BNL submission of 191,193Ir files for ENDF/B-VII, based on LANL files.
- Steven vdMarck says: 242,242mAm crashes in HEATR. Help resolve this – Bob MacFarlane didn't seem to have a problem (for Talou, MacFarlane, Kawano, Young).

Trellue

- Discuss with MBC doing 209Bi LA150 GNASH n,p induced calculations for B-VII – we forgot this isotope.
- Help check (with Talou) BNL 191,193Ir complete files that use LANL data, for B-VII.

Hale/Page

- p+13C file apparently incomplete and crashes NJOY processing. What to do?
- STANDARDS/Pronyaev. Standards used in beta2, except for 10B nn' and n,tot. (Nobody saw this really as a problem – this inconsistency between standards and beta2).
- Discuss n+2D status with MBC, and help provide a paragraph on this issue of ang dist, for B-VII paper.

Bob Little

- Rh-103 – MCNP expung error –could it be that the file is too big somewhere? (Little and MacFarlane?)
- For the B-VII paper. A few paragraphs on data testing of the photonuclear data, with a few figures showing the MCNP simulations v Barber and George data. Say for HEU, and for 1 or 2 other materials. Also, some text describing the (limited) DN testing we did, comparing results from 2 different spheres. (Little and White)
- Input to Skip. Re effort to include Madland's energy release in B-VII (set up a meeting with Madland, MacF, Little, Frankle, me, Young, etc to get this going & brainstorm)

Bill Wilson

- Steven vdMarck: B-eff. Calc using his own method, for reference calculations for fast & thermal systems. Fast range – look fine. In thermal case, beta-2 looks a bit high (say 5%) – JENDL3.3 looks better, and SVM thinks they were adjusted. Cecil says that a reduced delayed thermal 235U nubar will fix this.

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- Final response to Ridikas re his peer review and comments on 6th group of DN data,

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