IEC-191

Status Report for Subgroup 18 on U235 epithermal capture.

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June 13, 1998

For distribution at the Antwerp meeting of the WPEC, June 15-17, 1998

At the last meeting of the WPEC (Cadarache, May 1997) a comparison was made of the then-latest U235 evaluations from Oak Ridge and Harwell (Leal-Derrien-Wright May '97 and Moxon May '97). The L-D-W work incorporated integral data into the fitting process, a new capability of SAMMY, while Moxon, using REFIT, continued to work strictly with differential data, apart from his use of the CSEWG Standards Committee 2200 m/s values for fission and capture.

Despite this difference in approach, both evaluations produced excellent fits to most of the differential data, the result of a great deal of work with two powerful resonance-fitting codes. Although both sets were of an interim nature, the SAMMY runs produced complete ENDF-formatted files, while the REFIT results were well-converged up to 20 eV or so, so comparisons were limited to that region. There was a noticeable difference between the two evaluations in the shape of the capture cross section below 1 eV. The L-D-W set gave Westcott g-factors of 0.9883 for capture and 0.9776 for fission; Moxon's set gave 0.9507 and 0.9771. Thus the fission shapes were in agreement but the capture g-factors differed by 4%, a rather large amount for this important quantity. Another indication that more work was needed on the capture fitting was the peak capture at the 0.3 eV resonance, where the L-D-W value (50.6 barns) was 23% higher than Moxon's 41.2 barns.

It was not possible to resolve these issues at the meeting and the only action taken was to recommend that an attempt be made to reach a consensus before the October '97 CSEWG meeting. That turned out to not be feasible, and the two evaluation efforts are still separate.

The L-D-W set had been constructed to give acceptable thermal benchmark eigenvalues, as measured by the parameter K1. Its value (722.3) essentially guaranteed that. On the other hand, Moxon's set, which did not deal explicitly with nubar, implied a low K1 unless it could be coupled with a nubar higher than the ENDF/B-VI Standards value due to T. Axton (Reference 1). The accompanying table shows that with the ENDF/B-VI.3 value of 2.4338, K1 is 720.4, somewhat low. Higher nubar values exist in the measurements of Gwin, et al, and of Spencer, (Reference 2) both of which were part of Axton's least-squares fit, but which were reduced by the other data. The Gwin data, which are energy-dependent, have been adopted by both the current JEF and JENDL libraries. Using the JEF value (2.4374), Moxon's K1 is 722.3, quite reasonable. Allan Carlson pointed out that Spencer's value is even higher than Gwin's, and that Spencer has a high degree of confidence in the result. Thus, taking the numbers from Axton's report and the CSEWG Standards report, Gwin's 235/252 ratio (.64701) times the Standards 252 nubar (3.7676) gives 2.4377. The Standards 235 nubar (2.4320) "renormalized" by the ratio of Spencer's 252 nubar (3.7831) to the Standards value (3.7676) gives 2.4420. Unfortunately, there is no way to eliminate the low manganese-bath measurements and simply adopt the higher scintillator results, other than to argue that the benchmarks show a clear preference for the higher values. Incidentally, the "Spencer value" of 2.4420 would raise L-D-W May '97 from 722.3 to 727.0, and Moxon May '97 to 724.9. The former is high, but the latter would not be unreasonable.

To investigate this point, we put together a "tri-partite" deck, by inserting Moxon's fit from 0-10 eV into the January '96 ORNL data set, and replacing the nubar file with the JEF values. Benchmark testing showed that this hybrid set did well on the ORNL aqueous spheres, but poorly on the harder-spectrum cases. It appeared that the higher Gwin nubar was good for the soft-spectrum cases, but too high for the others. Because Moxon's data set was of an interim nature, the investigation was not carried further, but it raised the question (once again) of whether an energy-dependent nubar could resolve some of our differential-integral discrepancies.

In June of 1997, Dean, Hanlon and Perry (Reference 3) issued a report comparing eigenvalues as a function of spectral hardness for two calculational methods, five data sets, and ten benchmarks. They found general agreement between the preliminary data set (December '96) resulting from the ORNL-Moxon collaboration and Release 3, and in addition found very good results for the UH3-UR assembly with the December set. The results for the other two hard-spectrum cores UH3-NI and HISS were not as good as with the January '96 evaluation. These latter findings should be better understood, but that has not been done, because later versions were already available for testing. (Note: D-H-P showed that the nickel-reflected UH3-NI assembly cannot be calculated with multigroup cross sections, an effect noted earlier by RQ Wright at Oak Ridge.)

After Cadarache, Leal and Derrien, and Moxon continued to refine their fits, and released their current data sets in August and September of 1997. Relative to their May work, Oak Ridge moved toward less reactive shapes in the thermal region. As the table shows, their Maxwellian-averaged capture increased from 97.0 to 97.8 while the fission was essentially unchanged. To counteract this negative influence on K1, they increased nubar from the Release 3 value (2.4338) to 2.4367 over the range from 0 to 1 eV. They arrived at this value by treating thermal nubar as a search parameter in the SAMMY runs, while using the benchmark value of K1 (722.7) as a quantity to be fitted. The resulting value of nubar is close to a smooth average through the fluctuating Gwin data points, and fortuitously, it is exactly the ENDF/B-V value. In order to avoid the deleterious effect of a high nubar on the harder-spectrum cores, they linearly ramped nubar back down to the lower Release 3 value at 2 eV.

The necessity for such an approach is essentially forced on the evaluator who achieves a good fit to the differential cross sections, as both SAMMY and REFIT do. Over the years, successive refinements in fitting experimental data, made possible by the availability of more powerful computers, for example the use of multilevel formalisms, increased sophistication in the shape of resolution functions, more flexible renormalization methods, and multiple-scattering corrections, have failed to change the basic situation, which is that thermal benchmarks need a K1 around 723, and if the cross sections are accurately fit, a nubar of 2.4320 (Standards) or even 2.4338 (Release 3) is simply too low.

Upon release of the Leal-Derrien-Wright-Larson set in August, it was tested by A. C. Kahler (Bettis) and J. P. Weinman (Lockheed Martin-Schenectady), who obtained results for about 25 benchmarks, including ORNL spheres and cylinders, ORNL L-series, Rocky Flats, and 3 HISS(HUG) and UR3 intermediate-spectrum cases, using continuous-energy Monte Carlo codes. Their results were presented at the October CSEWG meeting and are available as Attachments 4-3 and 4-4 to the Minutes (Reference 4). They obtained results using ENDF/B-VI cross sections for the other materials in the calculations, and also for two "variant" cross section sets, for hydrogen and oxygen. The ENDF/B-VI results showed that the new L-D-W-L set gave integral (eigenvalue) results as good as Release 3, being on average only slightly low at the low-leakage end and rising slightly with leakage. Its advantage over Release 3 of course is that it fits the differential data better, replacing the average cross section adjustment procedure used in the former by the use of simultaneously-fitted integral quantities.

The variant hydrogen deck restores the 2200 m/s capture cross section to its ENDF/B-V value, 332.0 mb, from the slightly higher ENDF/B-VI value of 332.6. This raises the low-leakage cores 100 pcm on average, to a value which is essentially unity. Kahler presented experimental evidence in support of the lower value, and the change was adopted by CSEWG for Release 5. The other modification was in the oxygen, where an evaluation done at Lockheed Martin-Schenectady was used. This work, which will be presented by E. Caro at the October '98 Islandia ANS Conference, gives somewhat more forward-peaking in the angular distributions than ENDF/B-VI, with increased leakage. The result is a 100 pcm decrease (on average) at the high-leakage end, which together with the hydrogen change produces a very flat trend line. The oxygen modification was not adopted by CSEWG, because G. Hale at Los Alamos is currently re-evaluating the oxygen data and it was decided to wait for this to be finished.

The intermediate-spectrum cases are close together at about 1% high. The thermal cases are therefore about the same as Release 3, while the 3 harder cores are better. As a result of these findings, the L-D-W-L August '97 evaluation was adopted for ENDF/B-VI Release 5. The latter was intended for issuance in early '98 but is delayed by some formatting problems unrelated to the cross sections. The cross sections are available from Oak Ridge or Brookhaven. The tight grouping of the HISS / UH3 results differs from the result reported in Reference 3 and mentioned above, which of course used different data and different codes.

In December of 1997, two papers were presented at a meeting of the JEF Working Group on Data Evaluation and Benchmark Testing (Reference 5). Both showed significant improvements using L-D-W-L over the JEF-2.2 data set, which is similar to ENDF/B-VI Release 2. The studies covered a wide range of quantities, among them buckling measurements, k-infinities, temperature-dependent Westcott g-factors, and spent-fuel analyses. In each area the L-D-W-L set improved the calculation/experiment agreement. Of particular interest were the spent-fuel results, since they test the cross sections in a way that is relatively independent of any problems with nubar. As a result of these favorable findings, the new data were adopted for JEF-3.0.

Moxon's latest work is available from the Nuclear Energy Agency Data Bank at Paris and is described in Reference 6. It extends his earlier work to 130 eV, and achieves good fits to the differential data using a single value of the radiation width, close to the 38.2 mV he recommended in Reference 7. Above 130 eV he uses an earlier ORNL parameter set which fits the transmission and fission reasonably well. As of this date, Moxon's new data have not been reviewed or benchmark tested, since that will require them to be coupled with a nubar file and higher energy cross sections. If it is to be useful in integral calculations, it will probably require a new treatment of nubar, a topic for further investigation, as is the significance of his unusual Westcott g-factor for capture, noted above in connection with his May '97 work. At the present time, Moxon's fit is to the resolved-resonances only, and uses a J-dependent scattering radius. That option is allowed in the ENDF Generalized Reich-Moore (also known as Generalized R-Matrix) format, but not in the old Reich-Moore format. Since GRM has not been implemented in NJOY, there is a processing problem, but pointwise cross sections can be obtained from Moxon or NEA. Moxon has also worked on the unresolved region with a multilevel ladder-sampling technique but the results are not yet available. They show promise of being able to achieve a higher epithermal alpha in a region where intermediate-spectrum cores could be favorably impacted. Moxon has pointed out that the detailed fits obtained by the latest SAMMY and REFIT runs differ in the wings and valleys of the resonances. This needs to be further examined, but it is reasonable to assume that such differences could be induced by the incorporation of integral data into the fitting process, since normally the uncertainties on the differential data are largest in these regions. Another difference between Moxon's fits and those of L-D-M-L is in the average radiation width over 0-100 eV, which is 38 mV (a constant) in the former and 40 mV with a 10% standard deviation in the latter. One could speculate that the integral data are influencing this result, and that future changes in nubar might affect the L-D-M-L value. When the full 0-2250 eV region is included, the L-D-M-L value increases to 43 mV, one of the reasons we need an objective assessment of the pseudo-resonances in ENDF/B-VI (See point 2 in the next paragraph).

Looking ahead, it appears that further refinements in the U235 cross sections will require some new approaches:

1. Since the cross sections have been studied exhaustively, more attention should be focussed on nubar. Fission theory says that nubar will vary from resonance to resonance, so it is possible that incorporating a theory-based energy-variation of nubar into the resonance-fitting process could further improve both the thermal and intermediate-spectrum calculations. A new measurement, directed specifically at the energy-variation of nubar, may be advisable.

2. We need an improved representation of the unresolved resonance region. A way to get at this area might be to set up a realistic set of fictitious pointwise cross sections in an accurately-specified fictitious geometrical model, and use monte carlo to calculate detailed reaction rates. While these would be fictitious values, they would provide a calculational benchmark against which multigroup codes could be tested. In the current ENDF format the most potentially-serious deficiencies are the use of a single-level Breit-Wigner formalism and the lack of a way to properly treat inelastic competition. More sophisticated aspects of fission theory, such as the inclusion of barrier and channel effects should also be looked at.

This could answer a related question, whether some difficulty with the absorption rate in U238 is due to data or the self-shielding methodology. The point is important if a U238 problem is obscuring errors in the U235 in LEU assemblies. Recent indications are that accurate point-energy monte carlo calculations may be giving good U238 results (Reference 8).

On the same topic, an answer is needed to the question of whether the "pseudo-resonances" in ENDF/B-VI U235 between 150 (or so) eV and 2250 eV are better or worse than a treatment using average unresolved parameters. For this purpose also, a fictitious, but accurately specified calculational benchmark, coupled with monte carlo probability tables and an accurate multilevel URR treatment, could provide an answer.

3. It is possible that the difference between Moxon's current thermal-region capture shape and L-D-W-L would produce an observable effect in the analysis of an experiment that was sensitive to the hardness of the thermal spectrum, such as the moderator temperature coefficient work which led to drooping eta.

4. Finally, it would be interesting to put accurate numerical "worths" on some of the solid-state effects which Moxon believes he has seen in his work, such as non-free-gas broadening and Bragg scattering. Unfortunately, the cost / benefit ratio on these is likely to be much higher than the previous topics, as would their practical implementation in real-world reactor caclulations

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(References 1-8 were mentioned in the preceding text. The others are included here because they cover topics related to the work of the Subgroup)

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CROSS SECTIONS AND OTHER PARAMETERS FOR SOME U235 EVALUATIONS

Version name	V#	SIGC	GCAP	MAXC	SIGF	GFISS	MAXF	0.3 CAP	0.3 FISS	NUBAR	K1	RIC	RIF	EPITH. ALPHA
Standards	--	99.0	.9902	98.0	584.3	.9771	570.9	----	----	2.4320	719.5	------	------	------
Reynolds	60	97.9	.9813	96.1	585.2	.9736	569.8	48.2		2.4349	721.5	135.3	272.9	.496
ENDF/B-V	68							48.3		2.4367				
ENDF/B-VI.1/2 (1)	67	98.8	9895	97.8	584.5	9786	571.9				722.2			
ENDF/B-VI.3/4 (2)	89	98.6	.9897	97.6	584.8	.9786	572.3	44.4		2.4338	723.0			
L-D-W 1/96	97	98.8	.9888	97.7	584.5	.9790	572.3			2.4320	721.8			
L-D-W-M 3/97	100	99.0	.9913	98.1	584.5	.9797	572.6	----	----	2.4338	722.9	139.8	276.8	.505
L-D-W 5/97	101	98.1	.9883	97.0	584.5	.9776	571.4	50.6	192	2.4338 2.4420	722.3 727.0			
MOXON 5/97	102	99.5	.9507	94.6	581.6	.9771	568.3	41.2	189	2.4338 2.4374 2.4420	720.2 722.3 724.9			
MOX 5/97 + LDW 5/97 + JEF v	105	99.5	.9492	94.4	581.6	.9777	568.6	41.2	189	2.4374	722.9	142.8	274.1	.521
ENDF/B-VI.5 L-D-W-L 8/97	107	98.7	.9911	97.8	585.0	.9765	571.3	46.5	194	2.4367	722.9	140.5	276.0	.509
MOXON 9/97	108	98.3			581.7			48.6	197	-------	------	------	------	------

Notes:
(1) ENDF6.2 did not change the cross sections.
(2) ENDF6.4 corrected an error in the prompt nubar file in Release 3.