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Summary Record of a NEACRP Restricted Specialists' Meeting on the Intercomparison of methods for calculating shielded Cross Sections in the Unresolved Resonance Region

Santa Fe, USA, Wednesday 15th May 1985

Participants:			
	E. Fort	CEN Cadarache	France
	F. Froehner	KFK Karlsruhe	F.R.Germany
	P. Hemmig	DOE Washington	USA
	R. Hwang	ANL Argonne	USA
	R. McFarlane	LANL Los Alamos	USA
	C. Nordborg	NEA Data Bank	France (Secretary)
	P. Rose	BNL Brookhaven	USA
	J. Rowlands	AEEW Winfrith	UK
	M. Salvatores	CEN Cadarache	France (Chairman)
	G. de Saussure	ORNL Oak Ridge	USA
	M. Sowerby	AERE Harwell	UK
	H. Tellier	CEN Saclay	France

The meeting was opened by the Chairman, M. Salvatores, who welcomed the participants and introduced the two observers: S. Ganesan, India and W. Poenitz, USA. The reason for holding the meeting during the International Nuclear Data Conference in Santa Fe was that this conference provided the opportunity for European and American scientists to discuss progress and to review the results of the benchmark calculations performed so far.

J. Rowlands started the discussion by summarizing the progress made in the intercomparison exercise and presented results obtained for the first specified series of benchmark calculations. Three type of problems had been identified:

1. what calculation method to use in the unresolved resonance region,
2. how to compare results between resolved and unresolved calculations,
3. how to best represent the unresolved resonance region in the ENDF-V format.

Calculation methods

R. Hwang had performed calculations for the U-238 benchmark and made comparisons with P. Ribon. After a number of ambiguities have been eliminated in the practical use of the codes, there was excellent agreement (a) between different modules calculated with the Hwang's analytical method, and (b) between the Hwang's method and a calculation performed with a resonance ladder generated by Ribon with its own method and code. It was indicated that the analytical method would be less performant in the case of Pu-239 at 300 eV, where a large contribution to the integral comes from resonances out of the range.

R. McFarlane suggested that the different computational methods in the unresolved resonance regions should be compared by using the entire ENDF/B-IV files for U-238 and Pu-239 and then calculate the infinite dilute cross sections and shielding factors at 300 degree Kelvin and with a 1/ t weighting at the energies given in the file (E*). The background cross sections should be for U-238: 1000, 300, 100, 30, 10, 0 and for Pu-239: 1000, 100, 50, 10, 1. R. McFarlane offered to circulate these data for further comparisons.

Preliminary calculations performed in Los Alamos had shown that the different modules (UNRESR, UXSR and PURR) incorporated in the code NJOY for the unresolved resonance region, had given very similar results in the low energy region. The agreement was within 1 percent at 4 keV for U-238 and slightly worse agreement at 301 eV for Pu-239. Computer listings showing the results for the UXSR module was given to C. Nordborg for further distribution to J. Gonnord, Saclay, France.

The Karlsruhe code MIGROS-3 would only work on the KEDAK format and could thus not participate directly in the comparison exercise, but F. Froehner indicated that he would follow the development closely and probably perform calculations after translating the ENDF/B-IV files to KEDAK format.

The calculation method used by P. Ribon, Saclay, France, in his program was discussed, but it was not clear to all participants exactly how it worked and C. Nordborg was therefore asked to investigate if the computer code itself and the generated ladders would be available for distribution to R. Hwang and R. McFarlane.

The lack of good experimental self-shielding data to test the absolute accuracy of the calculations was also discussed.

Comparing results between resolved and unresolved calculations

It was generally felt by the participants that the problem of comparing results between calculations in the resolved and unresolved resonance region should be deferred to a later stage when the computational methods for the unresolved region agreed to an acceptable accuracy.

Format representation in the unresolved region

The only allowable format in the unresolved resonance region in the ENDF-V format is the Single Level Breit Wigner (SLBW) formalism. G. de Saussure suggested that a ladder representation of this region would be preferable when proper account could be taken of the large "hidden" s-wave resonances at high energies. This would be fairly easy for U-238 but would

cause problems for U-235 and Pu-239. One of the advantages of this representation would be the possibility to update the files easily when new information became available.

The conclusion of this discussion was, however, that the SLBW formalism would probably be used in the near future and that the evaluators would instead try to extend the resolved resonance region to higher energies.

In practice, the recommendation was made to extend the resolved range of future evaluations up to about 15 KeV for U-238 and up to about 1 KeV for Pu-239. The best way to reach this goal was indicated as being to supplement the experimental evidence for a number of well-defined resonances, with a ladder, generated according to a specified procedure and directly included in the evaluation. The increase in the number of resonances is worthwhile to reduce the ambiguities in the processing of the data.

Conclusions

Essentially the following conclusions were reached:

(1) The Hwang's analytical method to treat unresolved resonances is well established and can be used with confidence at energies E> 10-15 KeV for U-238 and > 1 KeV for Pu-239.

(2) The ladder generation technique developed by Ribon seems to be very attractive and should be documented. The code based on this method should be made generally available.

(3) Resonance self-shielding measurements are still needed to verify the absolute accuracy of calculations (in terms of s-1).

(4) The different algorithms implemented in the same code for dealing with unresolved resonance give very close results. Some additional evidence will be given by the proposed calculation. However, it was stressed that the comparison should not be among codes but among methods.

(5) The problem of data representation in the so-called unresolved resonance region is the crucial one.

A recommendation was formulated and agreed by the evaluators present at the meeting to extend the resolved resonance region for U-238 and Pu-239 using the existing experimental evidence, supplemented by a complementary ladder generation according to procedures to be specified and which should be left to the responsibility of the evaluators. Work done already in this field (like the Ribon approach) should be considered.