Future Evaluated Nuclear Data for Uranium 235 Progress Report Summarised by C J Dean

BACKGROUND Reported in July 1996

In the UK, the IMC has supported evaluation studies and benchmark assessments of U235 nuclear data. These studies are part of a continuing international effort through sub-group 18 of the OECD NEA Working Party on Evaluation Collaboration, which highlights capture cross sections in the resolved resonance region. Progress is monitored through CESWG in the USA and through JEF working groups in Europe. Initial UK results were presented, with others, at the July 1996 JEF meeting in Paris.

It was clear that the Leal, Derrien et al evaluation, released for assessment in January 1996, contained significant differences from the data in JEF2.2. It was also clear that the effect of the differences varied with spectrum hardness as measured by slowing down density (proportion of fission neutrons reaching 4eV).

Mick Moxon had examined the January 1996 Leal, Derrien et al evaluation using his REFIT code and issued a paper proposing improvements. In July his early re-evaluation had resulted in changed data between 4 and 22eV but even these had changed DIMPLE S01 K-effective by 0.1% and a HISS result by nearly 0.3%.

A sub-meeting of those directly involved took place at the JEF meeting and came to two overall conclusions:-

1. Further work was required and should be directed towards a single enhanced evaluation for inclusion in both European

(JEFF3.0) and American (ENDF) libraries. The Japanese (JENDL) project should be kept informed of progress.

2. A set of about 10 reference benchmarks should be assembled. These should cover the full range of intermediate spectrum and thermal assemblies of interest to thermal reactor physics and criticality. Calculations should be run with fine energy representation in reference codes.

Mick Moxon had used his REFIT least squares resonance analysis code to fit experimental data. Most modern evaluations in Europe and the US use Nancy Larson's SAMMY code. Mick's U235 work indicates differences between the codes which could affect future evaluation world wide. It was therefore a matter of some urgency to study the differences and make enhancements to the codes as deemed necessary.

Progress Since July 1996

September Evaluation

The initial IMC supported work planned to have an evaluation to 100eV completed in September 1996 together with a benchmark report. Mick Moxon's unclassified evaluation report (AEAT-0716) was issued internationally to describe a base for studies at ORNL. Unfortunately when the file was processed with NJOY, QA procedures highlighted unacceptable changes to the thermal cross sections and to the shape of η . It is pointless generating WIMS and MONK data until this is resolved. The benchmark studies have thus been completed without the September MOXON evaluation. Investigations into the changes at thermal energies will be included in planned extensions described next.

Study at Oak Ridge USA

The OECD-NEA arranged a collaborative study at Oak Ridge. In that regard M. Moxon is working at ORNL with the support of KAPL in the USA, the IMC in the UK, and the CEA in France. Mick Moxon started working with Nancy Larson, Luiz Leal, Herve Derrien at the beginning of October 1996. This work will result in the following deliverables:-

- 1. A package to automatically convert from REFIT input to SAMMY input, and vice versa, to facilitate future comparisons.
- 2. A report proposing future development of the SAMMY and REFIT codes.
- 3. A 235 U evaluation containing "resolved" resonance data extending above 100 eV.
- 4. A report on the evaluation.

Details of the thermal problem became apparent after the programme was designed. However it is hoped that the comparison of the REFIT and SAMMY codes will help solve this problem and that the solution will be included in the evaluation. Further it is hoped that proposals for developments (or not) of the unresolved resonance parameters will be included in the report.

Another result of this work could be to recommend improvements to the SAMMY and REFIT codes with some enhancement. Further development could be supported by student effort centred at Cadarache. The resultant code would be available for use in Europe and America.

Mick Moxon's visit to the US is scheduled to end in early December. Deliverables are targeted at the end of December.

Progress at the Beginning of December 1996

Benchmarking

NJOY91.91 has been used to process ²³⁵U evaluations, based on JEF2.2, ENDF/B-VI revisions 2 and 3 and the January 1996 Leal, Derrien et al evaluation, to produce group data for WIMS7 and MONK7.

A set of 10 suitable benchmark cases has been selected.

Calculations have been run with the MONK5W option of WIMS7 and with MONK7. The 172 group results compare well with those from the hyperfine (13,193 grouped) calculations with MONK7 for all but one case. This has a Ni reflector and the 172 group Ni data are known to be inadequate even when shielding is added. Results using resonance supplemented with the Leal, Derrien et al evaluation of 255 U are similar to those reported in the USA when the Leal, Derrien et al evaluation is used with ENDF/B-VI revision 3 except for one case with a natural Uranium reflector. Investigations are in progress. These results are not yet documented but will be reported at the December JEF Meeting.

After any comments at the JEF meeting this selection of benchmarks can be used to study the JEF3.0 ²³⁵₉₂U evaluation resulting from the Oak Ridge study.

OAK Ridge Study

Deliverables

- 1. A package to automatically convert from REFIT input to SAMMY input, and vice versa, to facilitate future comparisons. Several codes have been written and used. They are yet to be documented.
- 2. A report proposing future development of the SAMMY and REFIT codes.

A paper entitled "Doppler Broadening Revisited" has been issued to CESWG and will be available at the December JEF meeting. Results from REFIT, SAMMY and NJOY are comparable at 0K. Differences at room temperature are mainly due to the use of an approximate Doppler model called High Energy Gaussian Approximation (HEGA). This was being applied by REFIT above 1eV for U235 but its application is being switched off. Similarly it can be turned on and off in SAMMY. The full model is recommended at all energies and is used by the latest version of NJOY at ORNL.

These conclusions have implications on many existing evaluations generated using the HEGA model both in ENDFB and JEF libraries. i.e. the evaluator used the HEGA model to fit measurements and obtained resonance parameters which are then used in the full model by NJOY.

3. A 235 U evaluation containing "resolved" resonance data extending above 100 eV.

A revision of the ORNL evaluation, constraining the values of the radiation widths to much smaller fluctuations, is being completed up to 500eV by L Leal, H Derrien, N Larson and M Moxon using SAMMY and REFIT. A mean capture width - Γ, of between 38 and 40 meV fits all but about 7 resonances (below 100eV) seen from transmission and fission measurements. This topic is still under investigation. REFIT is being used to check the SAMMY evaluation and to study particular features.

The thermal fit is one of these features. Currently "back - scattering" from aluminium is being blamed. It could be possible that negative energy resonances were adjusted to compensate for a lack of scattering correction (seen in the background cross section between resonances) in some early SAMMY calculations. When the improved scattering was introduced in REFIT the negative energy resonances were left and hence over-compensated giving incorrect thermal cross sections and η shape.

REFIT calculations take a long elapsed time and will need to be completed when Mick Moxon returns to Harwell.

4. A report on the evaluation.

The evaluation and the report are expected to be available for consideration for possible inclusion in JEFF3.0 and ENFBVI revision 4 by the end of January 1997.

Reports to the UKNSF and JEF Meetings.

Mick Moxon had hoped to report to both meetings. However, there was clear need for as much collaborative work as possible. Since some estimates of expenses left funds remaining, it was thought better to spend these in consolidating the work in the USA.

Unresolved Resonance Data

M Moxon and L Leal (in consultation with C Durlston and others) started some studies of the unresolved region above 2.2KeV. Current results are showing about 30% differences in capture from ENDFB-VI (=JEF2.2) values when fission is adjusted to fit within a few percent. This region has particular impact on hard spectrum assemblies (e.g. HISS) where current Keff predictions are high.

Other Evaluation Related Topics

Mick Moxon has been asked to help in measurements of $^{233}_{92}$ U thermal and resonance data. He was also asked to continue the $^{235}_{92}$ U unresolved resonance range evaluation.

Interaction between resonances in some fission products (%Te, 133 Cs, 147 Pm) 234 U, 236 U and 238 U, particularly close to 6.7 eV resonance in 238 U, seems to be important yet it is not considered in most US and UK codes.