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EVALUATED NUCLEAR DATA FOR TH-U FUEL CYCLE

Summary Report of the Third Research Coordination Meeting

IAEA, Headquarters

Vienna, Austria

30 January to 2 February 2006

Prepared by

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IAEA Headquarters, Vienna, Austria

February 2006

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

The work completed to date was reviewed and the necessary tasks for completion of the evaluated data files for ^{232}Th, ^{231,233}Pa, ^{232,233,234,236}U were assigned. The ^{232}Th and ^{231,233}Pa files will be offered for inclusion in the ENDF/B-VII library. The layout and the deadlines for producing the document describing the evaluations were defined. With the completion of the above listed tasks, the project will be closed.

February 2006

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Introduction

The meeting was opened by A.L. Nichols, Head of the Nuclear Data Section who especially mentioned:

- importance of the final results for the implementation of the Th-U fuel cycle, e.g., in India,
- quality of the results already obtained that have been recognised by other projects such as the ENDF/B-VII project,
- existence of a CRP in which new experiments were carried out and analysed, as well as the evaluation of existing experimental data.

Nichols also mentioned that Trkov, the IAEA Scientific Secretary of this Coordinated Research Project (CRP), will retire from the IAEA in 2006. However, he hoped that Trkov would be able to continue to coordinate the CRP until completion.

Ignatyuk was elected Chairman of the meeting and Schillebeeckx agreed to be the rapporteur.

The agenda was revised to include the following presentations:

- Covariances in the resonance region by Leal.
- Evaluated nuclear data for the Th-U fuel cycle by Janeva.
- Th-U neutron data up to 200 MeV by Maslov.
- Fission Cross Section Measurements and Calculations for Pa Isotopes by Hambsch.
- Status of the covariance data by Kawano.

The revised agenda was adopted.

1. Status of the CRP

Trkov repeated the objective of the CRP, i.e., the production of documented and benchmarked evaluated nuclear data files of specific relevance to the Th-U fuel cycle (referred to as INDL/Th-U hereafter), and summarised the status of the project. The main achievements to date are:

- a full ^{232}Th evaluated file has been prepared and is ready for review and testing,
- preliminary ^{231,233}Pa full evaluated files have been assembled,
- the contributions for ^{232,233,234,236}U will mainly come from other projects, e.g., the Minsk file (prepared by Maslov) and ENDF/B-VII.

The Minsk ^{232}Th evaluation, which is a possible alternative to the joint evaluation, has been updated. For more details about the individual data files in the INDL/Th-U library, refer to the presentation of Trkov. He discussed the strong and weak points of the files produced within the CRP and suggested further work on the following:

– Improvements to neutron emission spectra.
– Small improvements of models for odd nuclides.
– Completion of work on cross-section covariance data.

Finally, Trkov mentioned the following points that should be the subject of this meeting:

– endorse proposed deliverables or choose alternatives,
– define scope of additional work and assign tasks,
– define time frame for the final delivery of all outputs and closure of the project.

2. ^{232}Th evaluated data file

2.1. Resonance region

Resolved resonance region

Leal described the file for the resolved resonance region which extends up to 4 keV. The file includes a full covariance matrix and reproduces the thermal total and capture cross sections. A large number of fictitious p-wave resonances have been included on the basis of resonance statistics. He specified the data which were analyzed and stressed the importance of the n_TOF data for the shape of the capture cross section in the eV region.

In the second part of his presentation, Leal discussed the production of the covariance data for the resolved resonance region (RRR). He summarized the status of the processing codes for the covariance data in RRR:

- NJOY is not capable of processing Reich Moore covariance data.
- PUFF has been developed at ORNL to process Reich-Moore covariance data.
- ERRORJ processes most of R-matrix covariance files.

He presented some benchmark calculations of the ICSBEP handbook (KBR-18,19,20,21) done with the KENO code, and results of sensitivity studies with the TSUNAMI code.

An extension of the RRR to higher energies would be desirable, but not possible with existing experimental database. Corresponding measurements are recommended.

Unresolved resonance region

Schillebeeckx presented the history of the evaluation in the unresolved resonance range (URR), which is based on an energy-dependent scattering radius. The energy dependence mainly compensates for the contribution of the external levels. The average resonance parameters were obtained from a simultaneous fit to the experimental data, applying a generalized single level representation with width fluctuations. However, not all processing codes can handle the energy-dependent scattering radius (only RECENT has this capability; PURR module of NJOY cannot even handle multi-range representations), even though the energy-dependent scattering radius is an accepted ENDF format. The adopted solution was to put pointwise cross-section data in ENDF file MF3 and use the same resonance parameters, but with a fixed scattering radius. With a constant scattering radius corresponding to energy 4 keV, the self-shielding factors were verified to remain the same to within 0.1%. This ensures that there is consistency of both the cross sections and the self-shielding factors compared to the results that are obtained with the energy-dependent scattering radius. The cross sections (total, capture and in-elastic scattering) of the analysis with the energy-dependent scattering radius are fully consistent with those of EMPIRE calculations.

The agreement between the experimental data, in particular the capture and inelastic, and the results of EMPIRE were discussed in several sessions:

- most of the apparent differences in the capture data are within 2 standard deviations,
- the high value of the experimental inelastic cross section at 144 keV by Fujita could be due to the fact that the data were measured at a Si-filtered neutron beam.

Janeva presented the work done at INRNE for ^{232}Th in the resolved and unresolved resonance region:

- resonance analysis in the RRR is finalized - the results were obtained from a simultaneous analysis of the n-TOF capture data, ORELA transmission data and the capture and transmission data of the IRMM using REFIT,
- results obtained with the new version of the HARFOR code, which includes an improved understanding of the external level contribution, are consistent with the cross sections in the Th file - this good agreement can be considered as an important validation of the results in the URR. Unfortunately, the HARFOR approach is not yet part of the ENDF format and is not implemented in existing processing codes.

Recommendations:

- effort should be made to implement the HARFOR approach in the ENDF format and the processing codes,
- the average parameters obtained with the HARFOR code should be reported in the file,
- the importance of the results obtained with the HARFOR code for the evaluation in the URR should be mentioned in the file.

2.2. Evaluation above the resonance region

Capote presented the results for the fast region obtained with EMPIRE using the dispersive coupled-channel optical model potential, a consistent treatment of the neutron emission and the triple humped fission barrier. He showed an extensive comparison with experimental data up to 60 MeV. The following conclusion can be drawn:

- for the total cross section, there is a complete consistent description of the experimental data,
- BROND inelastic cross section data differ from the EMPIRE evaluation and the Minsk library above 10 MeV due to a lower estimate of the direct contribution to high-lying inelastic levels in the BROND evaluation,

- direct contributions of DWBA calculations within the EMPIRE framework for individual levels above 500 keV excitation energy are different compared to the soft rotator calculations by Maslov for the Minsk data file. However, average contributions from groups of levels are in agreement with available experimental data in both cases,
- the high energy tail in the (n,2n) cross section is lower in the present evaluation, compared to the BROND and Minsk file (discussed in section 2.4.),
- in the double-differential cross sections (DDXS), disagreements for emission energies between 2 and 7 MeV are observed, especially for high incoming neutron energies - this problem is strongly related to the problem of pre-equilibrium contribution to the high energy tail of the (n,2n) excitation function,
- the fission cross section is well described,
- also the proton and alpha production cross section are in good agreement with the available experimental data, although deuteron and triton productions are not included.

After the presentation of Capote, the results of the different available evaluations in the fast region were compared. From this comparison and various discussions (e.g. see also Section 2.4 on benchmarks) it was concluded that with a minor revision of the emission spectra the EMPIRE evaluation can be recommended.

2.3. Nu-bar and fission spectra

Before going into the details of the nu-bar and fission spectra, Ignatyuk presented the results of the BROND-3 evaluation and made a general comment on the good agreement between the different evaluations, particularly for the total and capture cross sections. The largest differences are observed for the (n,2n) reaction, where the pre-equilibrium processes are responsible for the differences. The (n,2n) cross section above 14 MeV in the BROND and Minsk evaluations favours Butler's measurement (1961) at 18 MeV in preference to Karius (1979), Prestwood (1961) at 16.5 MeV, and Butler at 20 MeV.

A description of the nu-bar with an accuracy better than 1% can only be obtained by fitting experimental data. Due to the lack of sufficiently accurate experimental data for ^{232}Th this is only possible below 7 MeV. Above 7 MeV, the data can be estimated from systematic fissilities of neighbouring nuclei. Above 20 MeV evaluations are based on theoretical models. However, some recent experimental data by Batenkov (2003) confirm the estimated nu-bars in the energy region between 50 and 100 MeV.

The average energies of prompt fission neutrons as a function of incident neutron energy for ^{235}U and ^{238}U show a clear dip around 7 MeV. Similar behaviour is expected for ^{232}Th, but has not yet been confirmed experimentally. A general agreement in the description of this dip exists in BROND and Minsk evaluations. However, substantial differences in prompt fission neutron spectra exist. These differences might be attributed to the pre-fission neutron spectra. Exclusive pre-fission neutron spectra were taken into account in the Minsk evaluation, in a similar manner to ^{238}U+n and ^{235}U+n. For incoming energies above 14 MeV, the contribution of pre-equilibrium processes gives an essential contribution to the increase of the average energies of emitted fission neutrons. Above 14 MeV, the anisotropy of the emitted fission neutrons should be included in the evaluation.

New measurements for fission neutron spectra are scheduled at IRMM. The results could remove existing contradictions between benchmarks and differential measurements.

Essential contribution of pre-equilibrium processes above 20 MeV is confirmed by experiments on charged-particle emission. The main features of the charged-particle spectra and production cross sections are taken into account consistently in the BROND-3 evaluation.

2.4. Benchmarking

Trkov presented the verification and validation of the ^{232}Th data file. The file was verified for processability with different utility and processing codes and compared to experimental data.

- ENDF Utility codes (CHECKF, FIZCON, PSYCHE) produce no important messages and warnings,
- generation of pointwise file and ACE library demonstrates processability,
- comparison plots with EXFOR data indicate that the cross-section data are representative of the experimental data on which the evaluation is based.

The validation of the file was mainly based on:

- criticality benchmarks from the ICSBEP handbook: KBR (6 cases), THOR (1 case) and SB-n (8 cases),
- the leakage spectrum measurements for a ^{232}Th sphere with a D-T 14 MeV and ^{252}Cf source performed at the Institute of Physics and Power Engineering (IPPE), Obninsk.

Concerning the benchmark data, we can conclude that a smaller spread of the k_{eff} predictions is obtained when the analysis is based on the new file. The major improvement is for the configuration which is sensitive to the resonance region.

The analysis of the ^{232}Th-sphere leakage spectrum was of special interest. Although with the present file the experimental data are well described, deviations in the energy region between 2 and 7 MeV identified a shortcoming in the neutron emission spectrum. From a comparison with results obtained with the BROND and Minsk neutron emission spectra, we concluded that the discrepancy is likely due to the (n,2n) reaction and pre-equilibrium neutron spectra in the present file.

Recommendation:

Improve the neutron emission spectra in the IAEA file. According to Capote, this can be done before the end of February.

2.5. Covariances

The covariance data for the resonance region were discussed by Leal in Section 2.1. Kawano presented his analysis of the total cross section using the SOK and KALMAN codes. The results are limited up to 20 MeV, but an effort will be made to extend to higher energies. The final covariance data on the total cross section will be submitted by the end of February and the data for the other reaction channels by April. The uncertainty on the total cross section is about 1%, and the data show a strong correlation between the lowest and highest point.

A full covariance analysis based on a different approach was presented by Ignatyuk:

- the uncertainty in the total cross section for ^{232}Th is slightly above 0.5% up to almost 150 MeV,
- the uncertainty in the capture cross section below 300 keV is about 2%,
- the same level of uncertainty is obtained for the fission cross section to at least 20 MeV,
- the uncertainty in the (n,2n) is about 5% below 12 MeV,
- the uncertainty in nu-bar as a function of energy is about 1% below 20 MeV.

The correlation matrix of Ignatyuk for the total cross section is in reasonable agreement with the results of Kawano.

Recommendations:

- To improve the accuracy for the ^{232}Th inelastic channels, new measurements are recommended.
- According to Ignatyuk, the accuracy in the ^{232}Th capture cross section (about 2% below 300 keV) is now better than for ^{238}U.

2.6. Adoption of the ^{232}Th file

Tasks that need to be completed before general release:

- Include the average resonance parameters obtained with HARFOR in the comment file.
- Improve the neutron emission spectra in the IAEA file (Capote and Sin, end of February).
- An attempt will be made to extend the data file up to 150 MeV (Capote and Sin).
- Complete the covariances for the total cross section and the other reaction channels (Kawano, Capote, Trkov).
- Ignatyuk will finish the covariance file in a 32 group structure for ^{232}Th (beginning of March) and ^{233}U (beginning of April).
- Compare the results of different approaches for the calculation of the covariance matrix: KALMAN, BROND and IAEA approach. Since it is difficult to compare covariance matrices with different group structure, the comparison will be based on cross section data averaged over a typical fission spectrum. This approach is similar to the calculation of resonance integrals in the RRR.

Release of the file for the ENDF/B-VII project

- The Th-U website will be opened to the public.
- To release the file for the ENDF/B-VII project, we need to have the cross-section data by the end of February. The covariance matrix can be delivered later.
- A suggestion was made to present a review of the final results of the project at the upcoming ND2007 Conference in Nice (France).

3. ^{231}Pa evaluated data file

3.1. Resonance region

Leal presented his recommendation for the ^{231}Pa resonance parameters. He reviewed the existing evaluated data and made a first selection of the resonance parameters by applying the following criteria:

- upper energy range of the resolved resonance region,
- a clear separation of spin assignment,
- comparison with experimental data.

Based on the comparison with experimental data, the parameters of Mughabghab were preferred to the JENDL3.3 data. Leal also performed a statistical analysis of the fission widths to complete the data file using an average value of the fission width. Leal will attempt to convert the MLBW parameters into the Reich-Moore formalism.

The Minsk file will be adopted which extends up to 70 keV for the URR.

The covariance data for the resolved resonance region may be generated by Leal.

3.2. Fast region

In the fast region Capote presented the results obtained with EMPIRE following the same strategy as for ^{232}Th:

– Except for ENDF/B-VI.8 (adopted by JEFF3.1), the other libraries produce similar total cross sections.
– For the (n,2n) reaction, the EMPIRE evaluation seems to be higher than other evaluations.
– The EMPIRE fission cross-section evaluation is based on the latest IRMM data (see presentation Hambsch). Other evaluations follow mainly the Plattard and Fursov data. There is a disagreement between the EMPIRE fission data and the current version of the Minsk file, which is due to different emissive and first-chance fission contributions. In the former case, it is supported by the experimental point around 14 MeV by Birgul and preliminary IRMM data between 15 and 21 MeV.
– In the low energy region, the fission cross section agrees well with the results obtained from a lead slowing down spectrometric study performed by Kobayashi.
– To fill the gap between 6 and 14 MeV, new measurements are recommended.
– For the prompt fission neutron multiplicity and in view of the absence of any experimental data, the simplest JENDL3.3 evaluation was adopted in EMPIRE. An attempt will be made to include a new evaluation of PFNM and PFNS provided by Hambsch.
– Maslov pointed out that the IRMM fission spectra are not taking into account consistently the contribution of pre-equilibrium neutrons. Maslov will improve the fission spectra in file 5 for ^{231}Pa up to 20 MeV, and will make adjustments at 20 MeV to take into account the spectra from IRMM.

The IAEA will also coordinate the assembly of the covariance data provided by Leal for RRR and by Capote, Sin and Trkov for the high energy region.

Ignatyuk noted that capture cross sections could be verified with results of integral measurements. In the BROND2 file, the capture cross section for ^{231}Pa was decreased by 50% for a consistent description of ^{232}U build-up in the BN-350 fast reactor. Ganesan proposed a PIE measurement be performed in India in the Fast Breeder Test Reactor to check the capture cross section of ^{231}Pa.

4. ^{233}Pa evaluated data file

4.1. Resonance region

Leal presented his recommendation for the ^{233}Pa resonance parameters. He reviewed the existing evaluated data and made a selection of the resonance parameters which was partly based on the same criteria as for ^{231}Pa.

The ENDF/B-VI , JENDL3.3, JEFF 3.1 and Mughabghab data were excluded due to the mixing of spin states and/or the limited energy range for the RRR. A MLBW resonance parameter file produced by Mourogovskij was suggested by Trkov. Although in this file the RRR extends up to 106.6 eV, the resonances have a mixed spin state. To solve this problem, Leal performed a statistical analysis to split the spin states. Subsequently, he transformed the MLBW into the Reich-Moore formalism, while ensuring consistency with the thermal total and capture cross section. Ignatyuk reviewed the resulting average resonance parameters and confirmed their consistency.

Leal also produced a covariance matrix for the RRR.

In the unresolved resonance region the average resonance parameters from the Minsk file were adopted, which extend up to 70 keV.

4.2. Fast region

Capote presented the results obtained with EMPIRE in the fast energy region, following the same strategy as for ^{232}Th:

- The total cross section is in good agreement with other libraries.
- The (n,2n) cross section for ^{233}Pa obtained with EMPIRE seems to be overestimated in comparison with other evaluations.
- The fission cross section follows the IRMM data.
- The capture cross section deviates from the recent capture data of Petit et al. However, these are surrogate measurements and might suffer from a normalization problem.
- For the prompt fission neutron multiplicity and in view of the absence of any experimental data, the simplest JENDL3.3 evaluation was adopted for the IAEA

evaluation. A new evaluation provided by Hambsch will be adopted for both PFNM and PFNS.

- Maslov pointed out that the IRMM fission spectra are not taking into account consistently the contribution of pre-equilibrium neutrons. Maslov will improve the fission spectra in file 5 for ^{233}Pa up to 20 MeV, and will make adjustments at 20 MeV to take into account the spectra from IRMM.

The IAEA will also coordinate the assembly of the covariance data provided by Leal for RRR and by Capote, Sin and Trkov for the high energy region.

4.3. Fission Cross Section Measurements and Calculations for Pa Isotopes and Fission Mulitiplicity and Spectra Calculations for Pa Isotopes

Hambsch presented new direct measurements and calculations of the fission cross sections for ^{231,233}Pa. The calculations are based on a double-humped fission barrier. The model was validated by data for ^{232}Th and ^{238}U. He compared his results with those obtained from transfer reactions, and made a comment on the systematic uncertainty related to data deduced from transfer reactions. He also presented the neutron multiplicity and fission neutron spectrum calculated within the Los Alamos model. He presented multiplicity results for ^{230}Th and ^{231,232,233}Pa and the neutron spectra for ^{232}Th and ^{233}Pa. Good agreement with experimental data for the spectra is obtained for ^{232}Th.

4.4. Th-U neutron data up to 200 MeV – independent evaluation

Maslov presented his results for the ^{233,235,238}U and ^{231,233}Pa isotopes in the fast energy region. A recent analysis of prompt fission neutron spectra of ^{235}U demonstrated the importance of pre-fission neutron influence. The same approach is applied in the Minsk files for ^{233}U and other nuclides of interest for the Th-U cycle.

Maslov has noted that in his calculations he was not able to fit simultaneously the experimental data for U and preliminary IRMM data for 231Pa(n,F), when fission probabilities of 231Pa and 230Pa are fixed by surrogate measurements of the fission cross section.

Updated ^{232}Th evaluation for the Minsk file was presented. The ^{232}Th cross section was recalculated from 4keV to 5 MeV and it well describes the available database, particularly the new data from IRMM, n_TOF, Poenitz (1978) and Anand (1989) data. Discrepancies with EMPIRE calculations below 50 keV and above 800 keV are noted. They can be explained by the use of different partial entrance channel contributions to the capture reactions.

Direct contributions to vibrational levels were considered by the soft rotator model. Differences from the EMPIRE approach are discussed in section 2.2.

Similarity of ^{237}U (n,F) surrogate data of Pettner *et al.* (2005) and ^{231}Th (n,F) data prediction was demonstrated in the presentation. These data might contribute to the understanding of the chance structure of ^{232}Th (n,F) cross section.

5. ^{232}U evaluated data file

We should certainly not recommend JEFF3.1 and JENDL 3.3. In the fast energy region, the inelastic scattering cross sections in these files are definitely wrong.

It was decided to adopt the Minsk file. The advantages compared to the ENDF/B-VII file are the Reich-Moore resonance parameters in the RRR and better neutron emission spectra.

No covariance data will be included for ^{232}U.

6. ^{233}U evaluated data file

Before comparing the status of evaluated data, we agreed that a serious problem would be created if we do not adopt a consistent data file, since any changes would affect the interpretation of benchmarks. Re-evaluating the data file would require the same effort as for ^{232}Th.

Since a lot of effort was put into the ENDF/B-VII evaluation and validation, it was proposed to adopt this file for the INDL/Th-U. However, we decided to include the prompt fission neutron emission spectra from the Minsk file. Maslov will document the differences in PFNS between ENDF/B-VII and the Minsk file, and Trkov will verify the impact of this approach for at least one fast assembly (JEZEBEL 233) and one thermal lattice.

The data for both the RRR and URR will be taken from ENDF/B-VII. The structure in URR is produced by applying resonance statistics to maintaining the average parameters. The data have been produced by Leal and are well documented.

The covariance data in the resolved resonance region will be provided by Leal. Unfortunately, covariances from ENDF/B-VII for the fast region will not be delivered within the time frame of this CRP.

An alternative file in the region up to 150 MeV is provided by BROND that will include the covariances of Leal in the RRR and independent evaluation for the fast energy region for the main cross sections. Benchmark validation of this file has not been done.

7. ^{234}U evaluated data file

There is a problem with the present evaluations due to a wrong interpretation of the experimental data. One of the authors (Harvey) of the experimental data recommends adopting the parameters that are listed in the publication together with 25 meV as an average radiation width.

Leal volunteered to transform these parameters into RM resonance parameters and adjust the bound state to the thermal cross-section values.

Kawano noted that the preliminary results of capture measurements at DANCE/LANSCE can only be described with an extremely small radiation width of 15 meV.

For the fast region, preference is given to the Minsk evaluation as compared to ENDF/B-VII because of a better description of PFNS (unless a re-evaluation would indicate some contradictions).

8. ^{236}U evaluated data file

It was decided to adopt ENDF/B-VII.

9. Delayed neutron data for ^{231,233}Pa

For ^{231}Pa, delayed neutron data are available. However, for ^{233}Pa no evaluated data file contains any delayed neutron data at all. Ignatyuk will provide delayed neutron spectra for ^{231,233}Pa in the 8 group approach by the end of March.

10. Fission product yield data

Liu Ping presented the status of the fission product yield libraries. The latest version of ENDF/B-VII and JEFF 3.1 fission yield libraries, together with the JENDL-3.3 and CENDL 2 data, were compared with each other and with experimental data. In the comparison, 3 fissile nuclides and 54 product nuclides were selected. For a quantitative assessment, the reduced χ^2 and the yield ratio (R) for each product nuclide and for each of the four libraries together with the average reduced χ^2 and ratio R were calculated. The smallest values were observed for the fission yields in the JEFF 3.1 library. Since the JEFF-3.1 library shows the best consistency with the experimental data for ^{232}Th and ^{233}U, and the better consistency for ^{235}U, the JEFF-3.1 fission product yields are recommended to be used for the Th-U data file. However, the JEFF-3.1 data must be improved for a problem which has already been pointed out in a previous report. According to Trkov, this problem has been solved by Mills. Liu Ping will verify if the problem has been resolved and will make corrections if necessary.

For several Pa isotopes, mass yield data are listed in the PhD thesis of Petit. Prof. Liu Tingjin will produce data for ^{231,233}Pa based on systematics.

For ^{232,234,236}U, Liu Ping together with Prof. Liu Tingjin will provide data from whatever library that has data available, preferably JEFF-3.1.

Action : Ganesan to follow all basic fission product yield measurements in India and organize their submission to EXFOR.

11. Integral validation

Ganesan presented a progress report on the creation of new Indian experimental benchmarks for integral validation of nuclear data for the thorium fuel cycle. It was pointed out that the new basic evaluated nuclear data files for major and minor isotopes of Th-U fuel cycle created by this CRP are important for the development of advanced nuclear systems in India utilizing thorium.

Permission to publish the data has been obtained. India shares its experimental information and is welcome to benefit from the developments related to the use of thorium around the world.

The uncertainty in the benchmark of KAMINI in characterizing the predicted k_{eff} is $\pm$ 0.00744 which is within the acceptable limit of 1%. A finalized version of the KAMINI benchmark of very high quality has been submitted, peer reviewed and accepted for inclusion in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP). The benchmark evaluation of KAMINI has been accepted in the 2005 ICSBEP handbook at the time of this CRP meeting, and is expected to be released as an internet version in the ICSBEP website soon after completion of final editing. Thus, India has formally joined the USDOE-NEA efforts as a contributor to the preparation of the ICSBEP handbook. See website of ICSBEP: http://icsbep.inl.gov/2005/ for details.

The evaluation of the Indian PHWR thorium PIE benchmark needs to be brought to a level of international quality. However, the finalization and completion of the task on Indian PHWR thorium irradiation benchmark, including a large number of sensitivity studies, will be very involved, and is expected to take a few more months to complete.

Recommendations:

At the moment no integral data for the PIE of thorium fuel irradiations are available; only the Indian experiments presented by Ganesan can be considered for future validation. Ganesan will continue the validation of the new CRP file on the basis of these benchmark experiments.

The KAMINI criticality ^{233}U fuelled benchmark (accepted by the ICSBEP) provides ideal integral data to test the ^{233}U cross sections in the thermal spectrum range in view of the high quality of this benchmarking. Leal offered to explore the possibility of performing sensitivity studies using ORNL capabilities based upon TSUNAMI and KENO codes. The KENO model of this benchmark is not yet available in the ICSBEP.

The proposed visit of the Brazilian scientist (Hugo M. Dalle) in February 2006 for two weeks to work with Ganesan at BARC will be utilized towards the specific objective of further improving the quality of the Indian Th-irradiation PIE-PHWR benchmark. Leal will interact with Ganesan on both the KAMINI and PIE-PHWR benchmarks using ORNL capabilities. Trkov will provide WIMSD libraries of the new data of the CRP. An action was put on Ganesan to prepare a preliminary analysis with existing WIMSD libraries (www-ns.iaea.org/wimsd/) for the Indian Th-irradiation PIE-PHWR benchmark, and provide a report by 14 April.

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12. Library and documentation

IAEA-NDL/THU was proposed as the name of the library. Considering existing nomenclature and compatibility with the nomenclature in other IAEA documents, it was found impractical to adopt the proposal. The official name of the library is “IAEA Nuclear Data Library for Thorium-Uranium Fuel Cycle” with the acronym INDL/Th-U.

The file will be placed on the webserver of the IAEA Nuclear Data Library for the Th-U fuel cycle.

The structure of the comments in the ENDF file will be:

- authors: IAEA CRP Th-U fuel cycle, coordinator A. Trkov
- sections describing different file segments:
    - title
    - main authors
    - description

The evaluated data files are due by the end of February 2006.

A technical document explaining the details of the evaluation will be produced. Responsibilities for different sections of the document are evident from Table 1.

The use of Microsoft Word as text processor was agreed.

Trkov explained the conventions related to official IAEA publications.

Table of contents and the skeleton of the report are due by the end of March 2006.

Final contributions are due by August 2006:

- assembly and formatting will be done at the IAEA,
- main text should provide the explanation of what has been done,
- report will be organized with chapters by isotope, subchapters by energy region or data type.

Description of the resonance data for each nuclide will be prepared by Schillebeeckx, Leal and Janeva.

Description of the covariance data will consist of several sections provided by different authors.

- methodology in RRR by Leal,
- methodology for ^{232}Th by Kawano,
- methodology of the IAEA by Capote,
- methodology at IPPE by Ignatyuk.

Before WPEC meeting (1 May 2006), a draft document on covariances should be delivered.

The description of the fission yields will be written by Ping.

The description of benchmarking will be the responsibility of Trkov, in coordination with Kawano.

- Trkov will also include new ENDF/B-VII in the benchmarking, provided that official ENDF/B-VII ACE files are available.
- Validation is isotope interrelated; for ^{233}U, only spot checks will be undetaken.

Ganesan will briefly describe benchmarking activities in India, making reference to the KAMINI benchmark, and present preliminary results of PIE data analysis (also indicating future activities in benchmarking and validation).

Table 1: Responsibility assignment for different chapters of the report.

	RRR	**URR**	**Fast**	**Cov. RR**	**Covariance Fast**
^{232}Th	Leal	Janeva, Schillebeeckx	Capote-Noy, Sin, Maslov, Ignatuk	Leal	Kawano, Iwamoto, Ignatuk, Capote-Noy
^{231}Pa	Leal	Maslov, Ignatyuk, Janeva	Capote-Noy, Sin, Hambsch, Maslov	Leal	Capote-Noy
^{233}Pa	Leal	Maslov, Ignatuk, Janeva	Capote-Noy, Sin, Hambsch, Maslov	Leal	Capote-Noy
^{232}U	Maslov	Maslov	Maslov	-	-
^{233}U	Leal	Leal	ENDF/B-VII , Maslov, Ignatyuk	Leal	Ignatyuk
^{234}U	Leal, Schillebeeckx	Maslov	Maslov	-	-
^{236}U	ENDF/B-VII	ENDF/B-VII	ENDF/B-VII	-	-

APPENDIX 13.1

International Atomic Energy Agency

Third Research Coordination Meeting on

"Evaluated Nuclear Data for the Thorium-Uranium Fuel Cycle"

30 January to 2 February 2006,

IAEA Headquarters, Vienna, Austria

Meeting Room A2774

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APPENDIX 13.2

International Atomic Energy Agency

Third Research Coordination Meeting on

Evaluated Nuclear Data for Th-U Fuel Cycle

IAEA Headquarters, Vienna, Austria

30 January – 2 February 2006

Meeting Room A2774

AGENDA

Monday, 30 January

08:30 – 09:30 **Registration** (IAEA registration desk, Gate 1)

09:30 – 10:00 **Opening Session**

Opening (A.L. Nichols)

Introductory remarks (A.Trkov)

Election of Chairman and Rapporteur

Discussion and adoption of the Agenda (Chairman)

10:00 – 11:00 *Coffee break and Administrative Matters*

11:00 – 12:15 **Session 1: Review of ^{232}Th evaluated data file**
(max. 10 min per presentation + 5 min discussion)

R.Capote Noy – model calculation

Luiz Leal/Peter Schillebeeckx – resonance evaluation

A. Ignatyuk/F.-J. Hambsch – nu-bar and fission spectra

A. Trkov - validation

General Discussion

12:15 – 14:00 *Lunch*

14:00 – 15:30 **Session 2: Adoption of ^{232}Th file**

Discussion on the general status of the file

- Resonance data (Leal, Schillebeeckx, Janeva, Gunsing)
- High energy data (Capote, Maslov)
- Covariance data (Leal, Kawano, Capote)
- Benchmarking (Trkov)

15:30 – 16:00 *Coffee break*

16:00 – 17:30 **Session 3: Adoption of ^{232}Th file** (continued)

Tasks that need to be done before general release

Release of the file for the ENDF/B-VII project

Tuesday, 31 January

08:30 – 10:00 **Session 4: Review of ^{231,233}Pa evaluated data files**

Current status of the files

L. Leal - Resonance parameters

R. Capote – Model parameters

A. Trkov – General status of file assembly

General discussion

10:00 – 10:30 *Coffee break*

10:30 – 12:00 **Session 5: Adoption/selection of ^{231,233}Pa files**

Tasks that need to be done before general release

Release of the file for the ENDF/B-VII project

12:00 – 14:00 *Lunch*

14:00 – 15:30 **Session 6: Adoption/selection of ^{232,233,234,236}U files**

Comparison with recent measurements

General discussion

15:30 – 16:00 *Coffee break*

16:00 – 17:00 **Session 7: Adoption of the full INDL library**

Tasks that need to be done before general release

Release of the file

- Web distribution
- Time frame.

19:00 *Social Event: Dinner at Restaurant Augustinerkeller*

Wednesday, 1 February

08:30 – 10:00 **Session 8: Special purpose files/extended validation**

- Fission product yield data (Liu Ping)
- Integral validation by benchmarking against post-irradiation examination (PIE) measurements (Ganesan).

10:00 – 10:30 *Coffee break*

10:30 – 12:00 **Session 9: Special purpose files/extended validation** (continued)

PIE benchmark development – status (Ganesan)

General discussion

12:00 – 14:00 *Lunch*

14:00 – 15:30	**Session 10: INDL library documentation**
	Scope
	Publication
	Task assignment
15:30 – 16:00	*Coffee break*
16:00 – 17:00	**Session 11: INDL library documentation** (continued)
	Task assignment
	General discussion

Thursday, 2 February

08:30 – 10:00	**Session 12: Drafting of summary document**
10:00 – 10:30	*Coffee break*
10:30 – 12:00	**Session 13: Drafting of summary document**
12:00 – 14:00	*Lunch*
14:00 – 15:30	**Session 14: Review of the summary document**
15:30	**Close of meeting**

GUIDELINES

General:

- Please, check the Th-U CRP web page “http://www-nds.iaea.org/Th-U/index.html frequently for announcements and up-to-date information.
- For all administrative queries please contact Ms. Janet Roberts on J.Roberts@iaea.org.
- For technical matters please contact the technical officer of the project Andrej Trkov on A.Trkov@iaea.org. with a copy to Ms. Roberts.

Presentations:

- The time for oral presentations at the meeting is deliberately short so that more time can be devoted to discussions.
- Background materials in electronic form can be sent in advance to be placed on the web.
- Any presentations should *not* describe details of the theoretical advances, but primarily inform the other participants (not necessarily experts in the field) of the status.
- Participants are expected to be familiar with materials placed on the web.

APPENDIX 13.3

TASK ASSIGNMENTS

Date	**Participant**	**Agenda no.**	**Task**
	Janeva	2.1.	elaborate on the HARFOR approach in the ENDF format and the processing codes.
20 February	Janeva	2.1.	prepare parameters obtained with the HARFOR code for inclusion in the comments of the Th file.
28 February	Capote/Sin/Trkov	2.4.	improve the neutron emission spectra in the INDL file.
28 February 15 April	Kawano/Capote/Trkov	2.5.	provide covariance data on the total cross section, and data for the other reaction channels.
1 April	Capote/Sin	2.6.	attempt to extend the data file up to 150 MeV.
15 March 1 April	Ignatyuk	2.6.	provide the covariance file in a 32 group structure for ^{232}Th, and ^{233}U.
20 April	Trkov	2.6.	compare the results of different approaches for the calculation of the covariance matrix: KALMAN, BROND and IAEA approach - the comparison to be based on cross section data averaged over a typical fission spectrum similar to the calculation of resonance integrals in the RRR.
1 March	Trkov	2.6.	make the Th-U website open to the public.
28 February		2.6.	release the file for the ENDF/B-VII project, (finalised cross-section data; covariance matrix can be delivered later).
28 February	Leal	3.1.	attempt to convert the MLBW parameter for ^{231}Pa into the Reich-Moore formalism.
28 February	Leal	3.1.	generate covariance data for the resolved resonance region of ^{231}Pa.
28 February	Capote/Hambsch/ Maslov	3.2. 4.2.	compare IRMM and Minsk PFNS spectra of ^{231,233}Pa for E‹20 MeV and possibly modify the IRMM PFNS and extend up to 60 MeV.

TASK ASSIGNMENTS cont'd

Date	**Participant**	**Agenda no.**	**Task**
28 February	IAEA	3.2.	coordinate the assembly of the covariance data provided by Leal for RRR, and by Capote, Sin and Trkov for the high energy region for ^{232}Th and ^{231,233}Pa.
	Ganesan	4.4.	propose PIE measurement to be performed in India in the Fast Breeder Test Reactor to check capture cross section of ^{231}Pa.
1 April 20 April	Maslov Trkov	6.	document the differences in PFNS between ENDF/B-VII and the Minsk file; verify, for at least one fast assembly (JEZEBEL 233) and one thermal lattice, the impact of changing PFNS for ^{233}U.
1 April	Leal	6.	provide covariance data for ^{233}U in resolved resonance region.
1 April	BROND	6.	an alternative file for ^{233}U in the region up to 150 MeV to be provided, to include the covariances of Leal in the RRR and independent evaluation for the fast energy region for the main cross sections.
1 April	Leal	7.	transform parameters (listed in publication of J. Harvey) into RM resonance parameters and adjust the bound state to the thermal cross section values.
31 March	Ignatyuk	9.	provide delayed neutron spectra for ^{231,233}Pa in the 8-group approach.
31 March	Liu Ping	10.	verify if the problem pointed out in a previous report on fission yields has been resolved by R. Mills and make corrections if necessary.
31 March	Liu Ping with Prof. Liu Tingjin	10.	provide corrected fission yield data for ^{232,234,236}U, preferably from JEFF-3.1 library.
1 July	Ganesan	11.	follow all basic fission product yield measurements in India and organize to submit the data to EXFOR.
1 July	Ganesan	11.	continue the validation of the new CRP file on the basis of benchmark experiments.

TASK ASSIGNMENTS cont'd

Date	**Participant**	**Agenda no.**	**Task**
31 March	Ganesan	11.	prepare a preliminary analysis with existing WIMSD libraries (www-ns.iaea.org/wimsd/) for the Indian Th-irradiation PIE-PHWR benchmark.
10 March	Trkov	11.	provide WIMSD libraries of the new data of the CRP.
	Leal	11.	interact with Ganesan on both the KAMINI and PIE-PHWR benchmarks using ORNL capabilities.
20 April		12.	release all evaluated data files.
31 December		12.	produce a technical document explaining the details of the evaluation.
31 March	IAEA	12.	prepare table of contents and skeleton of the report: - assembling and formatting, - main text to provide explanation of what has been done, - report to be organized by nuclides, then by data types(chapters by isotope, subchapters by region).
15 August	Schillebeeckx/Leal/Janeva	12.	description of the resonance data for each nuclide.
1 May 15 August	Leal Kawano Capote Ignatyuk	12.	draft document on covariances full desription of the covariance data: - methodology in RRR, - methodology for ^{232}Th, - methodology, - methodology.
15 August	Ping	12.	description of the fission yields.
15 August	Trkov in coordination with Kawano	12.	description of benchmarking: to include new ENDF/B-VII in the benchmarking, provided that official ENDF/B-VII ACE files available. for ^{233}U only, spot checks to be done.
15 August	Ganesan	12.	briefly describe benchmarking activities in India, making reference to the KAMINI benchmark and present preliminary results of PIE data analysis, indicating future activities in benchmarking and validation.

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