Minutes/notes from CM on benchmarking new CRP bDN data

13-15 December 2017, IAEA, Vienna

Participants: P. Dimitriou (Scientific Secretary), V. Piksaikin (IPPE), A. Sonzogni (BNL), R. Mills (NNL), M. Fallot (SUBATECH-Univ. Nantes), D. Cano-Ott (CIEMAT), D. Foligno (CEA-Cadarache)

Chair: A. Sonzogni, Rapporteurs: All

Presentations :

Piksaikin:

Fissioning systems: U-235_thermal, U-235_fast, U-238_fast, Pu-239_thermal, Pu-239_fast

CFY-libraries: JEFF-3.1.1, ENDF/B-VII.1, JENDL-4.0

Pn-libraries: P-K-M, Rudstam, E-W, Abriola & al. (2011), IAEA-2017

-upper/lower limits taken as nominal values; asterisks treated as nominal values; approximate values taken as nominal

Results of summation calculations of total delayed neutron yields (TDN) show overall increasing TDN, above the recommended values, except for fast U-238 where the new results (CFY from JEFF and Pn from CRP or P-K-M) agree with recommended values.

U235_thermal: With JEFF-3.1.1 CFYs the increase in the TDN is much smaller than when using ENDF/B-VII.1 or JENDL-4.0.

Pu239_thermal: JEFF-3.1.1 CFYs are the best for the TDN calculation.

Pu239_fast: ENDF/B-VII.1 CFYs are the best for the TDN calculation.

The recommended values come from experiments.

a) Validation of new Pn values against total delayed neutron yields (TDN) and <T1/2>:

-upper/lower limits taken as nominal values; asterisks treated as nominal values

Results show overall increasing TDN, above the recommended values, except for fast U-238 where the new results agree with recommended values.

No similar trend is observed in <T1/2> because of the normalization to the contribution/weight of the precursor to TDN. However, the fact that there is no observed decrease in <T1/2> whereas in some few cases there is an observed increase, suggests that the observed increase in TDN may be caused by the long-lived precursors.

b) systematics of <T1/2>

Based on compilation of experimentally determined (ai,Ti) for several fissioning systems: global systematics and systematics per element were obtained wrt (Ac/Z)·92. These systematics are compact and have good predictive power given that they are based on a larger experimental database. They can therefore be used to obtain ai and Ti for unmeasured fissioning systems.

Sytematics of abundances ai per group i for 8-group measurements for fast systems: also good predictive power.

Notes: half-lives Ti in 8-groups are fixed to SG6 recommendations for all systems; negative reactivity can be correctly reproduced using 8-group decay curves but not with 6-group; positive reactivity however well described by 6-groups as well.

Recommendation: present group-constants and <T1/2> systematics as an improvement over SG6 recommendations at CIELO meeting.

<u>Sonzogni:</u>

Balraj's tables need to be converted into entirely numerical tables: include Liso; %b for isomer; energy of isomer; symmetric uncertainties; Q-values; remove LaTex etc.

Results for TDN for thermal: overall increase, however uncertainties based on quadrature are small between 3.4-6.7%, while the single precursors' contributions are large. Uncertainties on the antineutrino yields are about 2% (too small). For limits took half the value with 50% uncertainty, while approximate and asterisks were taken as nominal values.

Most suspicious contributions: Rb-91, As-85.

The problem of treating uncertainties when calculating TDN for fissioning systems with hundreds of precursors needs to be solved: summation over quadratures of the relative uncertainties of the hundreds of precursors results in unrealistically small uncertainties for TDN. We need to find a solution to provide reliable uncertainties for use in the various applications (decay heat, anti-neutrino etc).

All new (T1/2, Pn) values will be incorporated into ENSDF and ENDF/B-8.1 in 2018.

<u>Fallot:</u>

Used MURE package (C++ interface to the Monte Carlo code MCNP. It is an open source) to calculate TDN and perform simulations of certain types of nuclear reactors.

Used the first version of Balraj's (April 2017) and observed same trend in resulting TDN values: larger TDN values.

IFY-library: JEFF-3.1. From the IFY she obtained the CFY

Pn-libraries: CRP and ENDF/B-VII.1

Interpratation of the CRP Pn-library: limits, *, and approx. are neglected and the nominal value is taken. However, Rb91 has not been considered (Pn=0) because the Pn value was only included in the comments of the April 2017 tables.

Simulation studies performed for LWR, FBR, PBR and MOX with TDNs from April 2017 tables: have obtained lists of important contributors and need to analyse them.

The uncertainty has been computed considering Pn uncertainties only (no contribution of the FY to the uncertainty). The conclusion is that the uncertainties are too small.

<u>Foligno:</u>

Performed summation calculations of TDN and <T1/2> using CFYs and IFYs with solution of time-evolution problem.

Interpretation of new CRP Pn Oct. 2017 tables: limits were treated in two separate calculations: min and max values.

Observed same trend in TDNs: larger values compared to JEFF-3.1.1 and ENDF/B-VII.1 even when using min values. Also found <T1/2> to be larger. Main culprit: 91Rb.

Comparison of Jeff-3.1.1 CFYs and equilibrium CFYs calculated with time-evolution starting from Jeff-3.1.1 IFYs: agreement to 0.004% for all except for 6 cases where disagreement varied from 0.4% to 33%. Tested with different decay data libraries but always got the same disagreement for the same seven cases. The cases are: Rb-96, Y-97m, Ag-120,124, In-133, Cs-144.

Fitted 8-group abundances to DN decay curve N(t) obtained from summation calculations using Oct. 2017 CRP tables: used resulting abundances to calculate activity and reactivity curves.

<u>Cano:</u>

Compared TDNs for all fissioning systems with FYs using different combinations of evaluated libraries: new CRP Pn tables give larger TDNs. Sometimes in worse sometimes in better agreement with recommended TDNs. When combined with Jeff-3.1.1 FYs the results are in better agreement overall.

Uncertainties are calculated using summation over quadrature: large contributions from FYs compared to Pns. Final TDN uncertainties are too small. Using Monte Carlo method cannot guarantee better results.

Do not observe differences in TDNs when using CFYs and IFYs + allowing them to decay to equilibrium, except for thermal U-235 (2%).

Benchmark: 8 fast systems and one thermal, all available in NEA Data Bank. General trend: new CRP PN tables lead to bigger discrepancies in beta_eff and k_eff for U-235 based fuel systems than for Pu-239 ones.

<u>Mills:</u>

No new results from last meeting, but comparing results from previous with Foligno showed agreement to major nuclides (although they were reported slightly differently). However, some differences for 96Rb, 97mY, 120Ag, 124Ag, 133In, 137I and 144Cs when Foligno compared CFY and IFY using the JEFF-3.1.1 DDL. The 137I appears to be due to an error reported in an Erratum to the JEFF report, but the others probably result from the JEFF evaluation. Mills agreed to investigate the JEFF releases to confirm the 137I corrected file was published on the web and to check whether the other differences required correction to either IFY or CFY. Mills to respond by end of Jan 2019 to confirm file to use. He also agreed to model the experimental results from Piksaikin using the final FY and ENDF/B-8+CRP DDL when data is available. Also will use GEF to generate thermal to 6 MeV FY for 235U and 239Pu and do TDNY calculations to compare with experimental energy dependence, both by end of March 2018, if CRP DDL is ready.

<u>Discussion</u>

Action on all: to agree on a definitive list of Pn values from Balraj's tables for use in practical calculations and provide an entirely numerical file to the users.

Action on all: repeat summation calculations for TDN and <T1/2> using this definitive list plus cumulative FYs from JEFF-3.1.1: this will allow for an internal inter-comparison of codes used for summation calculations with CFYs. The same has to be done for time-evolution codes starting from IFYs. These inter-comparisons should be discussed in the final publication (Nuclear Data Sheets).

Effort to produce a definitive list of Pn values for use in practical calculations lead to the following list of modifications that has been sent to Balraj, Iris and Libby for discussion and confirmation:

<u>List of modifications in adopted values tables to be used for practical calculations:</u>

All asymmetric uncertainties need to be symmetrized in the numerical file.

All limits need to be symmetrized in the numerical file.

How to treat combined values (*) from mixed sources in the numerical file: use the same values for g.s. and isomer but with 100% uncertainty. For instance, the Pn value for 98Rb GS will be 14.5 +- 14.5%, the same for the isomer. We will have to re-visit this problem together with experimentalists and evaluators on a case-by-case basis.

Approximate values (for T1/2): adopt value with 100% uncertainty.

More specifically the following modifications are recommended for the following nuclides:

Zn-83: remove limit ">" from adopted table and adopt as nominal value

Rb-91: Pn is now given as < 0.7%. It turns out that 91Rb has a large cumulative fission yield, so even a small Pn value can have an impact. Since the Q-value for Beta-n is about 130 keV, we expect this Pn to be around 10E-5%, so we recommended giving the value as "-", write in the comment "<0.7%", and use a systematic value in the numerical file.

In numerical file, limits need to be symmetrized:

Y-97 iso: Pn limit is kept in adopted table but symmetrized value is used in numerical file: 0.04+-0.04

Y-105: Pn limit is kept in adopted table but symmetrized value is used in numerical file: 0.41+-0.41

For the Molybdenum, Zr and Pd nuclides, measured Pn values tend to be larger than the global systematic values, we should perhaps consider giving the Pns as "+", with the measured values as comments and systematic values in the numerical files. At the very least, these actions should be done for 103Zr, 120Pd and comments should be written for the remaining nuclides indicating that the Pn values deviate from systematics, therefore we recommend that:

Zr-103: add "+" in adopted table and measured value in comments; replace with value from systematics in numerical file

Zr-104-107…: keep Pn limits in adopted tables but add comments that these values deviate from systematics; in numerical file use symmetrized values

Mo-109,110,111: add "+" in adopted table and move measured values in comments; replace with values from systematics in numerical file

Pd-120, 123: add "+" in adopted tables and move measured values to comments; replace with values from systematics in numerical file

Pd-121,122: keep Pn limit in adopted tables but add comment that the value deviates from systematics; use symmetrized values in numerical file

Pd-rest of isotopes: need to be checked again, disagree with systematics, have not been published in refereed journal only in PhD thesis; suggest they be removed from adopted table and add comments that they deviate from systematics; use values from systematics in numerical file

Ag: no recommendation yet for Ag-120, Ag-129 (g.s.)

The symbol ">0" allows for unphysical values, so we recommend replacing it with "+" in cases such as Cd-129 (g.s. and iso), Cd-133, Te-140. List value from systematics in numerical file.

Final recommendation for numerical file:

The final numerical file will have the following columns:

Nuclide name (character), Z (int), A (int), liso (int), Level Energy (double), ∆Level Energy (double), % beta-minus (double), ∆ % beta-minus (double), T1/2 (double), ∆T1/2 (double), P1n (double), ∆P1n (double), P2n (double), ∆P2n (double), P1n syst (double), ∆P1n syst (double).

Liso is the isomer count in the ENDF-6 format, liso=0 for the ground state, 1 for the first isomer and so on. The connection with the fission yields data is done through Z, A and liso. We need the level energy and %beta-minus for the isomers, otherwise we may not be able to obtain Qbn and T1/2.

Further actions:

Action on: IAEA to prepare the numerical file using input from NNDC on systematics. Deadline: 31 January 2018.

Action on: all involved to complete CFYs and IFYs summation calculations (except time-evolution) and submit results to coordinator (Mills). Deadline: 21 February 2018.

Action on: NNDC to prepare an updated ENDF/B-VIII.1beta decay data file. Deadline: 28 February 2018.

Action on: Mills, Fallot, Foligno to complete time-evolution calculations using new ENDF/B-VIII.1 decay data library. Deadline: 15 March 2018.

Final publication in Nuclear Data Sheets

In addition to the definitive numerical file, participants also discussed the content of the second part of the final document devoted to the Macroscopic Database. The sections were reviewed in detail and modifications were made accordingly. The revised outline is attached to this report.

Not to forget: 1st complete draft of document should be ready by **1st June 2018**.

Coordinators of final document should ensure that first drafts of sections are in *Overleaf* by end of April.

Some guidelines for preparation of final manuscript:

-avoid copy & paste of text from previous publications (own or other's)

-use Google Grammarly

-prepare figures following sample figure

-use last name of 1st author and year of publication for references, e.g. Piksaikin98, Piksaikin98a, Piksaikin98b

Outline of final report – 15/12/2017

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Coordinator: P. Dimitriou,
Contributors: B. Singh, I. Dillmann</td></tr>
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<tr><td colspan="2">Section 2: Methods and Measurements
Coordinators: J.L. Tain, K. Rykaczewski, I. Dillmann
Contributors: M. Madurga, R. Grzywacz, B.C. Rasco, A. Algora</td></tr>
<tr><td>2.1 Methods for measurements
(Rykaczewski)</td><td>2.1.1 Delayed neutron emission probabilities
Methods listed in reports (1 and 2-RCM, CM 2011)
(Rykaczewski, Algora, Dillmann)
Ranging-out: included under ion-gamma counting method (Rykaczewski)
Pure Gamma-counting (Algora, Lorusso)

What is needed: review pros and cons of each method

2.1.2 Delayed neutron spectra
He3 (Tain)
Proton recoil spectrometers (Tain)
TOF (Grzywacz, Madurga, Cano, Banerjee)

2.1.3 New methods
TAS – a comprehensive report on method (Tain, Rasco)
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CLYC (Cano)
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<tr><td>2.2 List of priorities for new measurements (Tain)</td><td>2.2.1 For Fission Reactor technologies based on inter-library comparisons of delayed neutron yields (Tain, Mills, Cano, Minato, Fallot):
List which isotopes have been measured, which not

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2.2.3 Anti-neutrinos (Fallot, Sonzogni)</td></tr>
<tr><td>2.3 New data (Dillmann): to contact all relevant parties</td><td>List of data measured and published since beginning of CRP (2013) – also not yet published-ALTO-Future measurements/what is left to be done</td></tr>
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Coordinator: B. Singh
Contributors: I. Dillmann, G. Mukherjee, X. Huang, McCutchan, Sonzogni, Liang, Birch, Chen, Miernik, Tain, Dimitriou</td></tr>
<tr><td>3.1 Compilation and evaluation methodology (Singh)</td><td></td></tr>
<tr><td>3.2 New evaluated data for Z=2-28 and possible updates for Z>28 (Singh)</td><td>Tables of recommended data and Q-values (AME2016); compilation tables in annexes</td></tr>
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3.4.2 Miernik (Miernik)

3.4.3 Kratz-Hermann?</td></tr>
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3.5.2 Evaluation of published spectra used as references for calibration purposes (Tain, Madurga)

Greenwood, Reeder, Kratz, Rudstam, incl. those in Brady’s thesis</td></tr>
<tr><td colspan="2">Section 4: Theory
Coordinator: I. Borzov
Contributors: T. Marketin, F. Minato, S. Chiba</td></tr>
<tr><td>4. Description of models (Borzov)</td><td>Overview of existing models (based on draft circulated at 3RCM incl. comparative tables)
Incl. FAM (Engel), new QPC models (Litvinova), Skyrme (Milano)</td></tr>
<tr><td></td><td>4.1.1 Self-consistent models (Borzov, Marketing, Minato)
-3 global: DF3+cQPRA, RMF, HFBCS+QRPA

4.1.2 Microscopic-Macroscopic
(Borzov,Marketin)
- Moeller et al 2012, Mumpower and Kawano

4.1.3 Macroscopic-Microscopic (Chiba)
- Gross theory</td></tr>
<tr><td>4.2 Comparison with new T1/2 and Pn tables</td><td>Annexes: include results in tables along with evaluated data: two tables for T1/2 and Pn respectively

Figs. In text</td></tr>
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<tr><td>4.3 Conclusions and recommendations: limitations, perspectives</td><td>Based on theory review in Appendix 2</td></tr>
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<tr><td colspan="2">Section 5: Measurements, analysis and compilation (10 pages)
Coordinator: V. Piksaikin
Contributor: F. Minato</td></tr>
<tr><td>5.1 Methods (Piksaikin) 5 pages</td><td>5.1.1 Delayed neutron yields (Piksaikin, Minato)

5.1.2 Delayed neutron integral spectra (Piksaikin)

5.1.3 Time-dependent parameters (Piksaikin)

Energy dependence

GEF calculations for U235, Pu-239 energy dependence from 0 to 6 MeV (Mills)</td></tr>
<tr><td>5.2 New measurements and compilation (Piksaikin) 5 pages</td><td>Covering all three above listed areas – mention future plans for measurements (IPPE, Cadarache)- 1 paragraph each</td></tr>
<tr><td colspan="2">Section 6: Basic summation calculations, uncertainty analysis and validation
Coordinator: R. Mills,
Contributors: A. Sonzogni, V. Piksaikin, D. Cano, M. Fallot, D. Foligno</td></tr>
<tr><td>6.1 CRP (T1/2,Pn) file for practical applications (Sonzogni)</td><td>Creation of a definitive numerical file of T1/2 and Pn values for use in applications spanning reactor technologies, anti-neutrino spectra and nuclear astrophysics</td></tr>
<tr><td>6.2 Delayed neutron yields Coordinator: Mills,
Contributors: Sonzogni, Cano, Piksaikin, Fallot, Foligno</td><td>Jeff-3.1.1 FYs, ENDF/B-8.0 + CRP Pn values using definitive numerical table
Jeff-3.1.1 FYs: Robert will check released version and send corrected one (137I)
6.2.1 Basic inter-comparison of nu-bars and main contributors for all systems using CFYs + IFYs (decay data JEFF-3.1.1; ENDF/B-VIII.0, ENDF/B-VIII.0+CRP (T1/2,Pn), CRP (T1/2,Pn))
For all fissioning systems

6.2.2 Inter-comparison for time-dependence for U-235 thermal; (decay data: ENDF/B-VIII.0+CRP (T1/2,Pn));
Specific conditions will be set after this meeting (Mills, Foligno, Fallot)

6.2.3 Comparison with recommended total delayed neutron yields from evaluated libraries-discussion on differences-identification of important precursors that give rise to the differences: use IFYs
Use decay libraries: ENDF/B-VIII.0+CRP (T1/2,Pn)</td></tr>
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	Fission systems: thermal U-235, Pu-239; fast U-235, 238: Th-232, Pu-239; U-233 Specific conditions for time-evolution calculations to be set after the meeting (Mills, Foligno, Fallot) **6.2.4** Uncertainty analysis on summation calculations using CRP (T1/2,Pn) values **(Cano)** Quadrature, Monte Carlo **6.2.5** Recommendations Describe problems in other FY libraries (e.g. 86Ge) and how it has been corrected, mention also other corrections in JENDL/JEFF etc
6.3 Delayed neutron integral spectra Coordinator: Piksaikin	Comparison of measured spectra with summation calculations using the ENDF/B-VIII.0+CRP (T1/2,Pn) tables for all systems with available data Internal comparison of calculations with Mills – Vladimir to provide irradiation conditions
6.4 Time-dependent parameters (Coordinator: Foligno, Contributors: Sonzogni, Mills)	From summation calculations: decay data ENDF/B-VIII.0+CRP(T1/2,Pn) For U-233 fast, 235 thermal and fast, 236 fast, 238 fast; Pu-239 thermal and fast; Th-232 fast; Am-241 fast, Np-237 fast Comparison with measured by Piksaikin (Foligno, Piksaikin) Uncertainty analysis with Monte Carlo (Foligno)
Section 7: Integral calculations- Impact of CRP (T1/2, Pn) on specific reactor designs Coordinator: D. Cano, M. Fallot	
7.1 Comparison with integral experiments (Cano)	Calculate and compare k_eff, beta_eff for 8 fast and one thermal systems
7.2 Study of impact of new CRP (T1/2,Pn) data on reactor calculations (Cano, Fallot)	liquid metal reactors, PBMR, FBR include sensitivity analysis
Section 8: Systematics of macroscopic DN data Coordinator: V. Piksaikin Contributors: A. Sonzogni, S. Chiba	
8.1 Time-dependent parameters (Piksaikin)	Formula + figures; <T1/2>
8.2 Delayed neutron yields vs degree of evenness of Z and N, mass asymmetry (Sonzogni, Chiba)	

Section 9: Recommended data Coordinator: V.Piksaikin	
9.1 Group constants (Piksaikin)	**Supply 6- and 8-group constants** (10 pages) Based on new experimental data appearing after WPEC/SG-6 for the whole set of nuclides that already have recommended data (WPEC/SG-6)
Section 10: Reference Database Coordinator P. Dimitriou	
10.1 Microscopic data	Retrieval interface, content, plotting and downloading tools
10.2 Macroscopic data	Retrieval interface, content, plotting and downloading tools
10.3 subsidiary databases (ENSDF, ENDF/B, JEFF, JENDL, ROSFOND, BROND)	Input from Mills, Sonzogni, Minato, Piksaikin
10.4 Beta-delayed neutrons in EXFOR	
Section 11: Conclusions Coordinator: Rykaczweski, Mills, Piksaikin	
Split into microscopic and macroscopic sections	-achievements of this CRP -limitations of current approaches -new detection and data acquisition technologies -needs for further developments for applications (SG, innovative reactors/ADS, assay of nuclear materials, nuclear astrophysics)