On the International Radiation Characterization Benchmarks Experiment Project (IRCBEP): User´s Point of View

O. Cabellos
oscar.cabellos@upm.es

INDUSTRIALES
ETSII | UPM

Consultant Meeting on the IRCBEP, IAEA´s Headquarters, Vienna, Austria. August 6-9, 2018

Outline

1. The necessity of Nuclear Benchmarks
2. Handbooks for ND B&V
3. Purpose of these Handbooks
4. Content of Experimental Handbooks
5. The need of IRCBEP: Identifying quantities
    - 5.1 Integro-Differential Verification and Validation
    - 5.2 Maxwellian-Avg. n-Induced Cross-Sect, KADoNIS
    - 5.3 s0 and Q0 values, Kayzero library
    - 5.4 Resonance Integrals
    - 5.5 Decay Heat and Inventory predictions
    - 5.6 Other Experimental Data
6. Conclusion

1. The necessity of Nuclear Benchmarks

- The necessity of nuclear benchmarks

- Nuclear Safety
  - Safety Assessment
  - Safer Operation
  - …

- Computational methods
  - Code verification
  - Cross-section data

ND evaluation projects utilize benchmarks on:

- Criticality -> **ICSBEP**
- Shielding/transmission -> **SINBAD**
- Reactor Physics -> IRPHEP
- Spent nuclear fuel - > SFCOMPO
- …
- Others

1. The necessity of Nuclear Benchmarks

❑ B&V of ND trough databases … JEFF Project

OECD BETTER POLICIES FOR BETTER LIVES — Nuclear Energy Agency — NEA NUCLEAR ENERGY AGENCY

B&V/WG

- Introduction
  - Past and recent B&V
  - Participants
- **B&V neutron cross-sections**
- B&V other nuclear data
- B&V covariance data
- Agenda
  - 1st B&W JEFF WG
- Conclusion

B&V of neutron XSs through NEA Databases

- Spectral average cross sections (Thermal,…, MXW, ^{252}Cf/ ^{235}U fission, …, integral resonances, … MACS,…)
  - EXFOR
- Criticality
  - ICSBEP/DICE
  - IDAT/IRPhEP
- Kinetics (βeff,…), spectral indexes
  - ICSBEP/DICE
  - IDAT/IRPhEP
- Transmission and Shielding
  - ICSBEP
  - SINBAD
- Burnup
  - Depletion: SFCOMPO
  - Reactivity: IRPhEP (EPRI program)

 5

Source: JEFF/DOC-1729. "Introduction to JEFF/WG on B&V". O. Cabellos (2015)

INDUSTRIALES
ETSII | UPM

2. Handbooks for ND B&V

Project	International Project	Official Activity at …
ICSBEP => DICE tool	**International Criticality Safety Benchmark Evaluation Project** https://www.oecd-nea.org/science/wpncs/icsbep/	WPNCS …. **The Working Party on Nuclear Criticality Safety (WPNCS)** WPEC …**Working Party on International Nuclear Data Evaluation Co-operation (WPEC)** ○ **SG45** "Validation of Nuclear Data Libraries (VaNDaL) Project" ○ **SG40/CIELO, SG39/SG46,…**
IRPhEP => IDAT tool	**International Reactor Physics Experiment Evaluation Project** https://www.oecd-nea.org/science/wprs/irphe/	WPRS … **Working Party on Scientific Issues of Reactor Systems (WPRS)** ○ WPEC …**SG33/SG39/SG46**
SINBAD => NEA tool ?	**Shielding Integral Benchmark Archive and Database** https://www.oecd-nea.org/science/wprs/shielding/	WPRS … **Working Party on Scientific Issues of Reactor Systems (WPRS)** WPEC …**WP on International ND Evaluation Cooperation (WPEC)/SG47** "Use of Shielding Integral Benchmark Archive and Database for ND Validation" ○ **SG40/CIELO, SG39/SG46,…**
SFCOMPO 2.0 => SFCOMPO	**Database of measured isotopic concentrations of spent nuclear fuel, with operational histories and design data** https://www.oecd-nea.org/sfcompo/	WPNCS… **Expert Group on Assay Data of Spent Nuclear Fuel (ADSNF)**
EXFOR => IAEA tools => NEA tools	**An extensive compilation of experimental nuclear reaction data** https://www-nds.iaea.org/exfor/exfor.htm	IAEA/NDS …**The International Network of Nuclear Reaction Data Centres (NRDC)** NEA/DB …. **JANIS Software**

3. Purpose of these Handbooks

The purpose of these Handbooks can be summarized:

- **Compile benchmark-experiment data into standardized format** that allows analysts to easily used the data to validate calculational techniques and cross-section data
- **Evaluate the data and quantify overall uncertainties** trough sensitivity analysis
- **Streamline the necessary step of validating** computer codes and nuclear data with experimental data.

  e.g. develop models (reference/detail) with verified magnitudes
- **Preserve highly valuable experimental data**

4. Content of Experimental Handbooks

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

Example: ICSBEP

Quality & Assurance

- thorough internal review
- independent peer review

5. The need of IRCBEP: Identifying quantities

The need of a database on **Radiation Characterization Benchmark Experiments**:

- Identifying quantities (not yet included in B&V) for "**Radiation Characterization"**

  - σ_0 thermal cross sections (2200 m/s)
  - RI
  - K0 - standardisation method of Neutron Activation Analysis (NAA)
  - Q0 =I0/ σ0

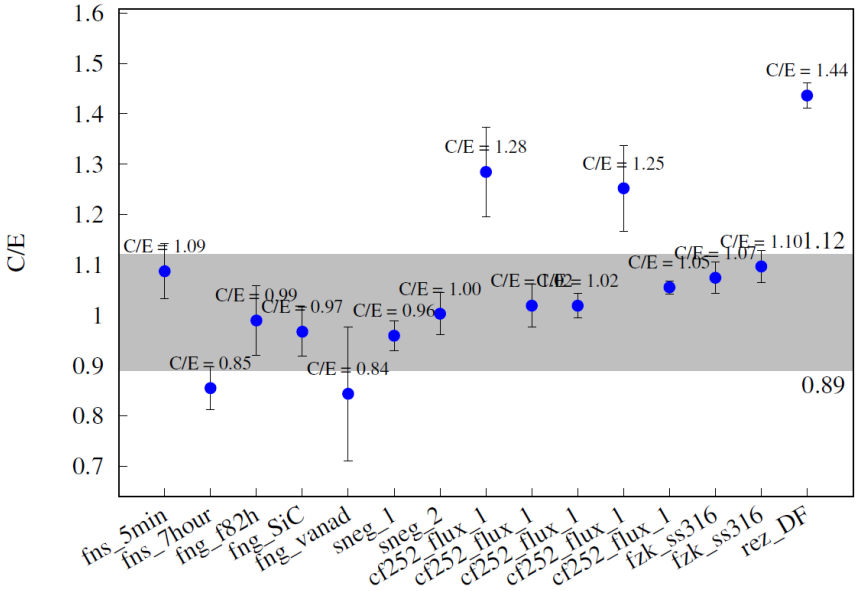
  - σ_th - spectrum-average thermal cross sections
  - Westcott g-factor

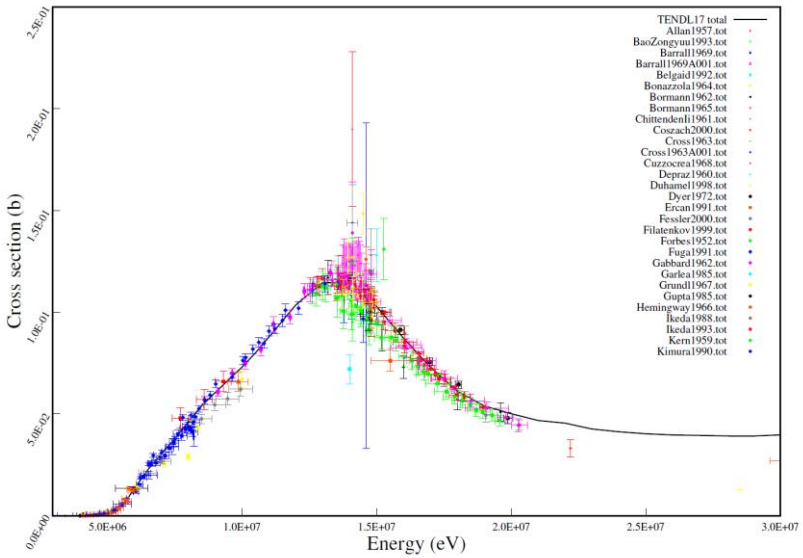
  - σ_14 MeV
  - MACS - Maxwellian Averaged Cross Sections
  - ...

5.1 Integro-Differential Verification and Validation

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Integro-Differential Verification and Validation**





Source: UKAEA-R(18)004. February 2018

Californium-252 spontaneous fission data ← **already in EXFOR**

5.1 Integro-Differential Verification and Validation

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Integro-Differential Verification and Validation**

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

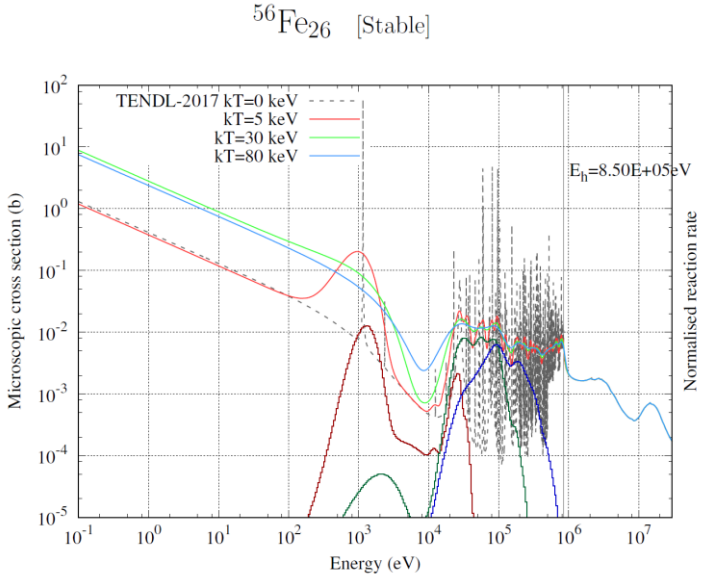
Procedure:

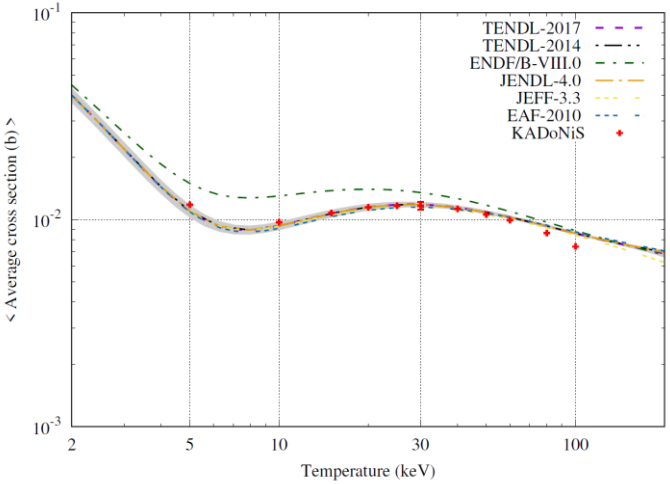
- Exp. Data:
  - EXFOR data
  - Others Exp: JAEA,TUD,…
- PREPRO/NJOY codes
- Database: Neutron Spectra
- Calculate: C+ΔC

5.2 Maxwellian-Avg. n-Induced Cross-Sect, KADoNIS

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100keV, KADoNiS**





Source: UKAEA-R(18)005. February 2018

5.2 Maxwellian-Avg. n-Induced Cross-Sect, KADoNIS

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100keV, KADoNiS**

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

Procedure:

- Exp. Data:
  - EXFOR data?
  - Others Exp: KADoNiS
- PREPRO/NJOY codes
- MAXWAV code ?
- Calculate: C+ΔC

5.3 σ0 and Q0 values, Kayzero library

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Comprehensive list of more than 100 reaction cross sections suitable for the activation technique: thermal cross sections (s0) and Q0 values**

2.5.20. $^{63}Cu(n,\gamma)^{64}Cu$

The thermal cross sections and the Q_0 values are as follows:

Mughabghab [1]			Kayzero [2] / Nudat [3]		JENDL-4.0 [4]		ENDF/B-VII.1 [5]	
σ_0	$\Delta\sigma_0$	Diff.	σ_0	$\Delta\sigma_0$	σ_0	Diff.	σ_0	Diff.
[b]	[%]	[%]	[b]	[%]	[b]	[%]	[b]	[%]
4.50	0.4	-2.7	4.624	1.1	4.508	-2.5	4.471	-3.3

Mughabghab [1]			Kayzero [2]		JENDL-4.0 [4]		ENDF/B-VII.1 [5]	
Q_0	ΔQ_0	Diff.	Q_0	ΔQ_0	Q_0	Diff.	Q_0	Diff.
	[%]	[%]		[%]		[%]		[%]
1.104	1.7	-3.1	1.14	-	1.087	-4.6	1.086	-4.7

Source: INDC(NDS)-0693

The measured values in the Kayzero library
http://www.kayzero.com/

5.3 σ0 and Q0 values, Kayzero library

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Comprehensive list of more than 100 reaction cross sections suitable for the activation technique: thermal cross sections (s0) and Q0 values**

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

Procedure:

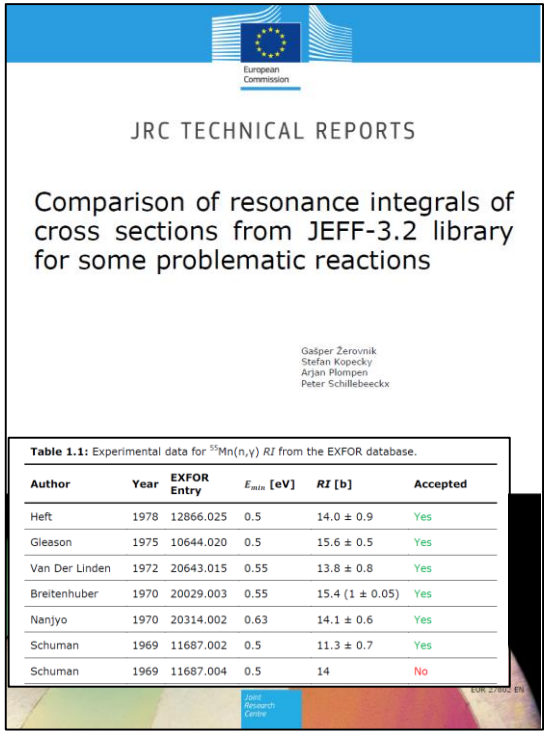
- Exp. Data:
  - EXFOR data
  - Others Exp: Kayzero library (A.Trkov)
- PREPRO/NJOY codes
- Calculate: C+ΔC

5.4 Resonance Integrals

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Resonance Integrals…. data in EXFOR**

Source: JRC report



European Commission

JRC TECHNICAL REPORTS

Comparison of resonance integrals of cross sections from JEFF-3.2 library for some problematic reactions

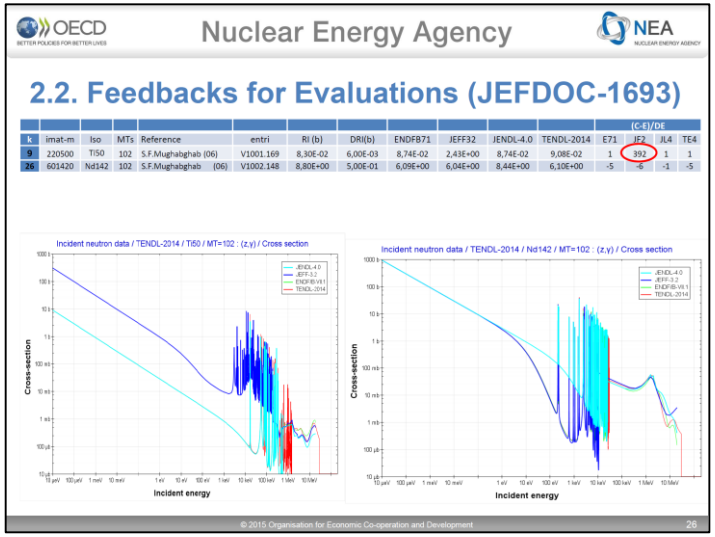
Gašper Žerovnik
Stefan Kopecky
Arjan Plompen
Peter Schillebeeckx

Table 1.1: Experimental data for ^{55}Mn(n,γ) *RI* from the EXFOR database.

Author	Year	EXFOR Entry	E_{min} [eV]	*RI* [b]	Accepted
Heft	1978	12866.025	0.5	14.0 ± 0.9	Yes
Gleason	1975	10644.020	0.5	15.6 ± 0.5	Yes
Van Der Linden	1972	20643.015	0.55	13.8 ± 0.8	Yes
Breitenhuber	1970	20029.003	0.55	15.4 (1 ± 0.05)	Yes
Nanjyo	1970	20314.002	0.63	14.1 ± 0.6	Yes
Schuman	1969	11687.002	0.5	11.3 ± 0.7	Yes
Schuman	1969	11687.004	0.5	14	No

Joint Research Centre

Report on Integral Resonances: A comparison between EXFOR and ENDF/B-VII.1, JEFF-3.2, JENDL-4.0 and TENDL-2014.
O. Cabellos, OECD NEA/DB. NRDC Meeting 2015.



OECD Nuclear Energy Agency NEA

2.2. Feedbacks for Evaluations (JEFDOC-1693)

k	imat-m	Iso	MTs	Reference	entri	RI (b)	DRI(b)	ENDFB71	JEFF32	JENDL-4.0	TENDL-2014	(C-E)/DE E71	JE2	JL4	TE4
9	220500	Ti50	102	S.F.Mughabghab (06)	V1001.169	8,30E-02	6,00E-03	8,74E-02	2,43E+00	8,74E-02	9,08E-02	1	392	1	1
26	601420	Nd142	102	S.F.Mughabghab (06)	V1002.148	8,80E+00	5,00E-01	6,09E+00	6,04E+00	8,44E+00	6,10E+00	-5	-6	-1	-5

5.4 Resonance Integrals

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Resonance Integrals…. data in EXFOR**

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

Procedure:

- Exp. Data: EXFOR data
- PREPRO/NJOY codes
- URR/CALENDF code?
- INTER code
- Input data for INTER: Lower-Upper energy limits
- Calculate: C+ΔC

5.5 Decay Heat and Inventory predictions

The need of a database on **Radiation Characterization Benchmark Experiments**:

❑ Decay Heat and Inventory Predictions

➢ **Fission Pulse Decay Heat**

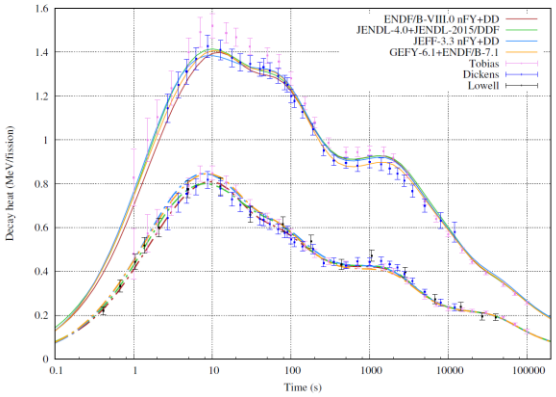
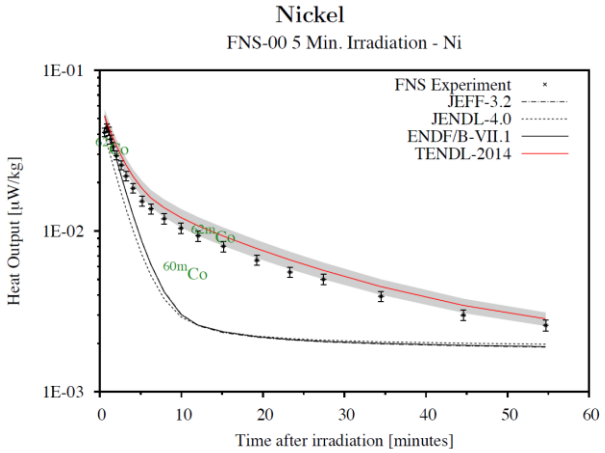


Figure 10: Total (solid) and beta (dash) decay heat from thermal pulse on ^{235}U.

"Meta-analysis performed by Tobias"

Source: UKAEA-R(18)003. February 2018

➢ **Decay Heat and Inventory Predictions**



"The lack of real chemical analysis of the irradiated samples, … (page 15)

Source: CCFE-R(15)25. January 2015

5.6 Other Experimental Data

❑ Integral experiments: Steel activation

7

PART I. Validation: integral activation experiments (FZKA-6764)

Table. Calculation-to-experiment average ratios for the activity inventories induced in the SS316 intermediate energy activation experiment FZKA6764

	IEAF2001	EAF2005			IEAF2001	EAF2005	
Isotope	C/E	C/E	Rel Err %	Isotope	C/E	C/E	Rel Err %
Sc 46	1.66	2.46	10.8	*Ni 57*	*1.19*	*1.22*	*0.5*
Sc 48	1.28	1.74	15.3	Y 87m	0.07	0.15	77.3
V 48	2.72	1.28	29.6	Y 87	0.46	0.82	63.3
Cr 48	3.73	1.54	82.9	Y 88	1.00	0.61	25.4
Cr 49	0.82	0.71	3.8	Zr 86	0.03	0.03	73.7
Cr 51	1.00	1.09	3.3	Zr 88	0.99	0.45	9.2
Mn 52	3.13	1.31	26.8	Zr 89	1.20	1.48	5.4
Mn 54	*1.02*	*1.16*	*9.4*	Zr 97	0.03	0.02	3.0
Mn 56	*1.23*	*1.22*	*0.6*	Nb 90	0.58	1.80	34.2
Fe 52	1.44	4.34	19.9	Nb 92m	1.51	1.46	4.1
Fe 59	1.07	1.18	17.8	Nb 95	1.53	1.65	6.1
Co 55	2.12	1.45	64.1	Nb 95m	1.18	0.84	9.4
Co 56	2.98	1.31	27.7	Nb 96	1.65	1.88	8.5
Co 57	1.02	1.12	0.9	Mo 90	1.64	1.97	71.5
Co 58	*1.20*	*1.19*	*3.0*	Mo 93m	2.50	1.81	44.2
Co 60	*1.12*	*1.03*	*3.3*	Mo 99	1.18	1.29	1.7
Co 61	2.26	2.66	17.5	Tc 99m	1.19	1.30	1.4
Ni 56	1.57	0.37	45.2				

This steel has been irradiated during 7,525 s with a neutron flux of $4.10*10^{11}$ n/cm^2 s having a neutron spectrum very close to IFMIF

Conclusions:

- For the most important radionuclides to the total activity and contact dose rate (56Mn, 54Mn, 57Ni, 58Co and 60Co): reasonable agreement
- For the rest of isotopes, larger deviations of C/E from unity were found.

These discrepancies can arise from:
- the activation cross section library
- neglecting the sequential charged-particle reactions (C/E: V58~1.01, Mn52 ~1.08, Co55 ~0.95, Co56 ~1.07)
- uncertainties of initial composition

- Our results are in good agreement with those obtained by ALARA, ANITA and FISPACT codes

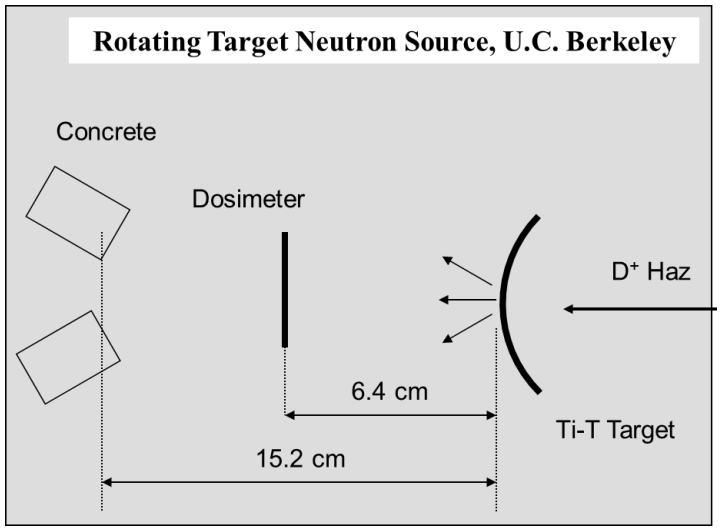
Source: EFFDOC-1101, "*Improvements in the prediction capability of ACAB code to transmutation Analysis in IFMIF*", O. Cabellos (2009)

5.6 Other Experimental Data

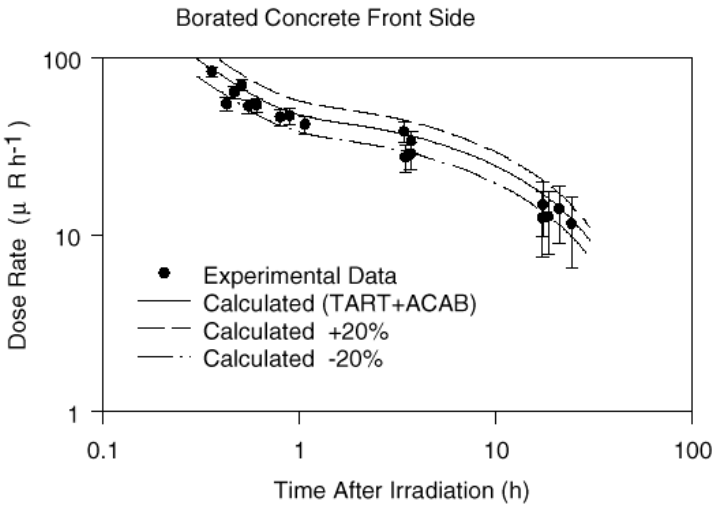
- **Integral experiments: Concrete activation**

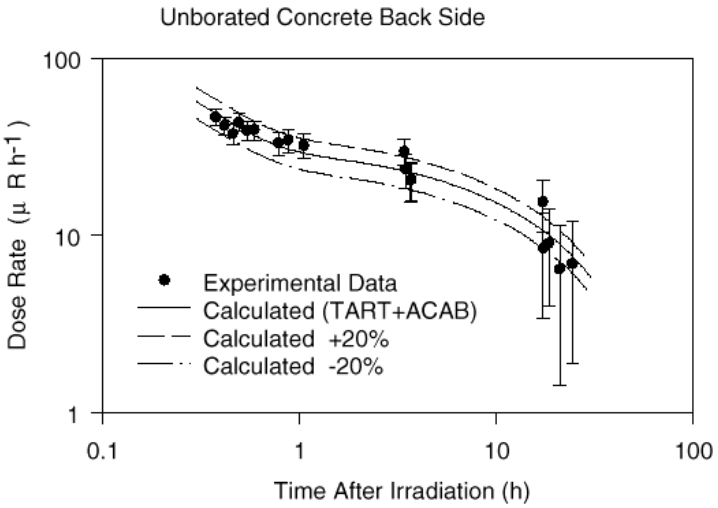
Source: ACAB Code Manual: Validation. (2008)

Source: "Experimental studies of concrete activation at the National Ignition Facility using the Rotating Target Neutron Source", A.P. Belian, J.F. Latkowski, E.C. Morse (1997) 17th IEEE/NPSS Symposium Fusion Engineering



Neutron intensity: 2.2 10^{10} n/s ± 20%
<E>= 15.2 ± 0.1 MeV
Irradiation time = 1h. 35 min.



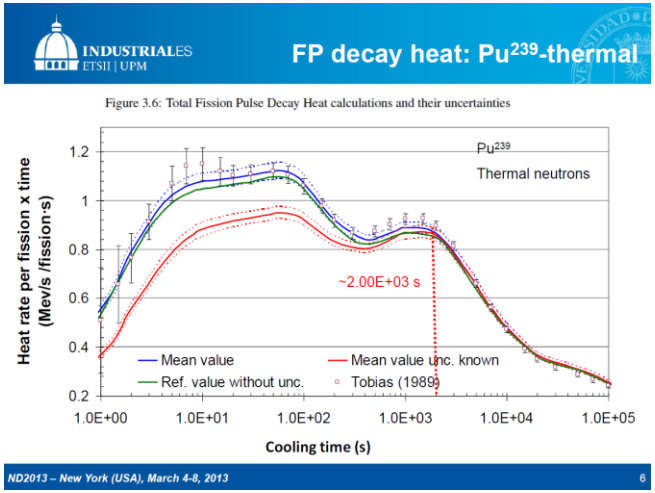


5.6 Other Experimental Data

- **FPDH**

"Comparison using Tobias data"

Source: ND2013, "*Testing JEFF-3.1.1 and ENDF/B-VII.1 DD&FY nuclear data libraries with Fission Pulse Neutron Emission and Decay Heat Experiments*", O. Cabellos et al. (2013)



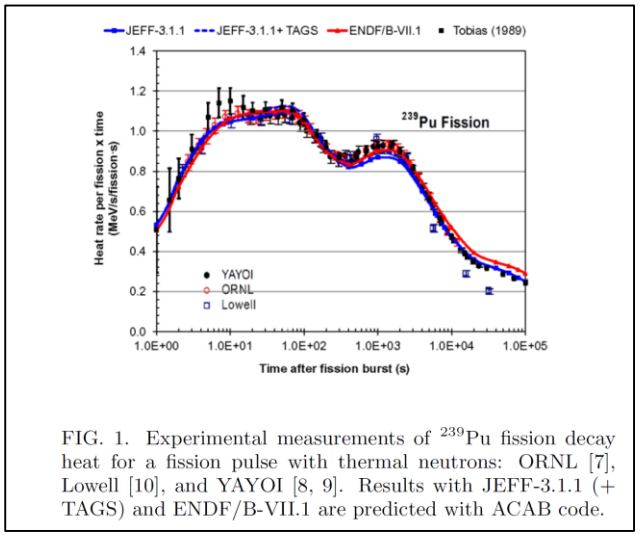


FIG. 1. Experimental measurements of ^{239}Pu fission decay heat for a fission pulse with thermal neutrons: ORNL [7], Lowell [10], and YAYOI [8, 9]. Results with JEFF-3.1.1 (+ TAGS) and ENDF/B-VII.1 are predicted with ACAB code.

"Meta-analysis performed by Tobias"

[6] A. Tobias, CEGB Report No. RD/B/6210/R89 (1989).
[7] J. K. Dickens *et al.*, Nucl. Sci. Eng. **78**, 126 (1981).
[8] M. Akiyama *et al.*, J. Atomic Ener. Soc. Japan **24**, 709 (1982) - in Japanese.
[9] M. Akiyama *et al.*, J. Atomic Ener. Soc. Japan **24**, 803 (1982) - in Japanese.
[10] W.A. Schier *et al.*, DOE/ER/40723-4 (1997).

"Experiments"

5.6 Other Experimental Data

- **Delayed neutron emission**

Source: ND2013, "*Testing JEFF-3.1.1 and ENDF/B-VII.1 DD&FY nuclear data libraries with Fission Pulse Neutron Emission and Decay Heat Experiments*", O. Cabellos et al. (2013)

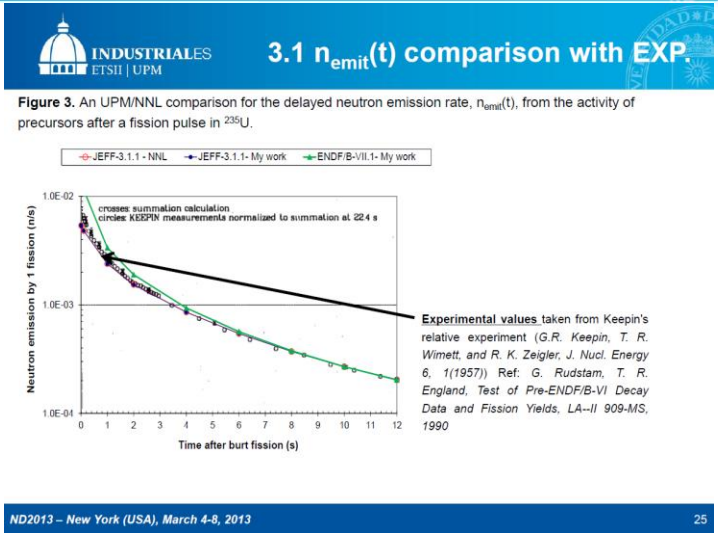


Figure 3. An UPM/NNL comparison for the delayed neutron emission rate, $n_{emit}(t)$, from the activity of precursors after a fission pulse in ^{235}U.

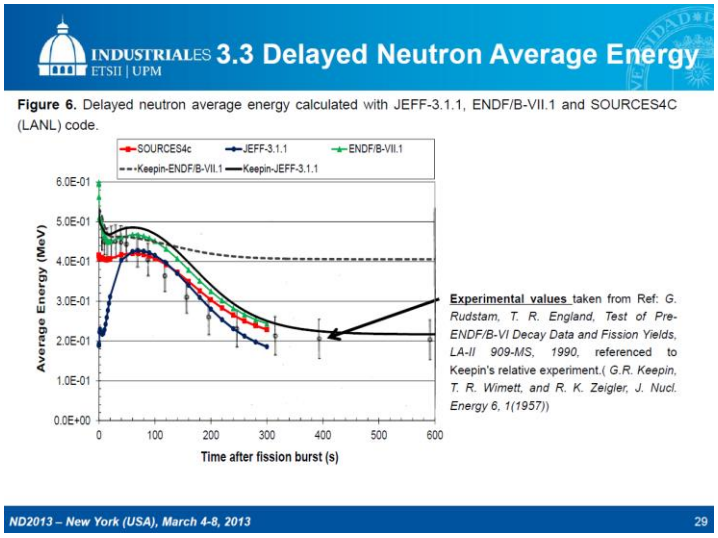


Figure 6. Delayed neutron average energy calculated with JEFF-3.1.1, ENDF/B-VII.1 and SOURCES4C (LANL) code.

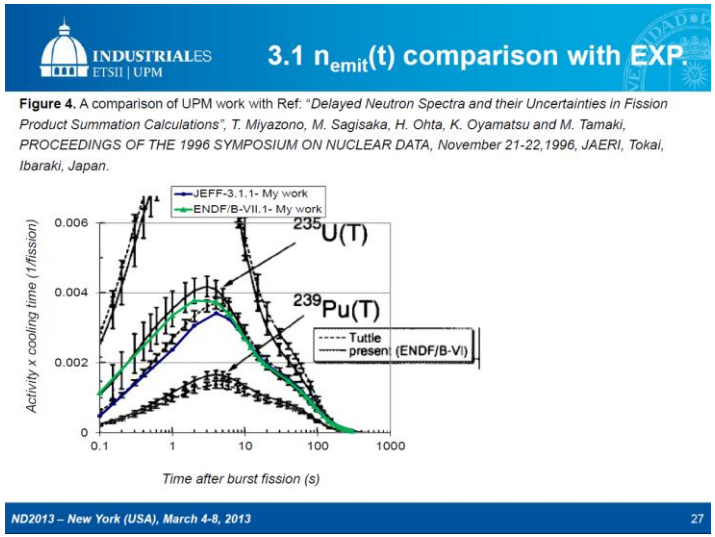


Figure 4. A comparison of UPM work with Ref: "*Delayed Neutron Spectra and their Uncertainties in Fission Product Summation Calculations*", T. Miyazono, M. Sagisaka, H. Ohta, K. Oyamatsu and M. Tamaki, PROCEEDINGS OF THE 1996 SYMPOSIUM ON NUCLEAR DATA, November 21-22,1996, JAERI, Tokai, Ibaraki, Japan.

5.6 Other Experimental Data

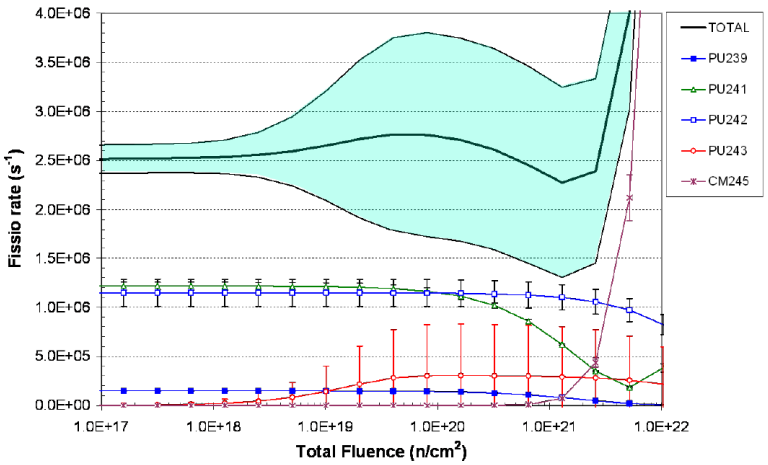
- **Other experimental data measurements ?**

Source: EFFDOC-1117, "*Assessment of **fissionable material behaviour** in fission chambers*", O. Cabellos (2010)

18

PART IV: Relative error in fission rates Pu242#1 in BR2

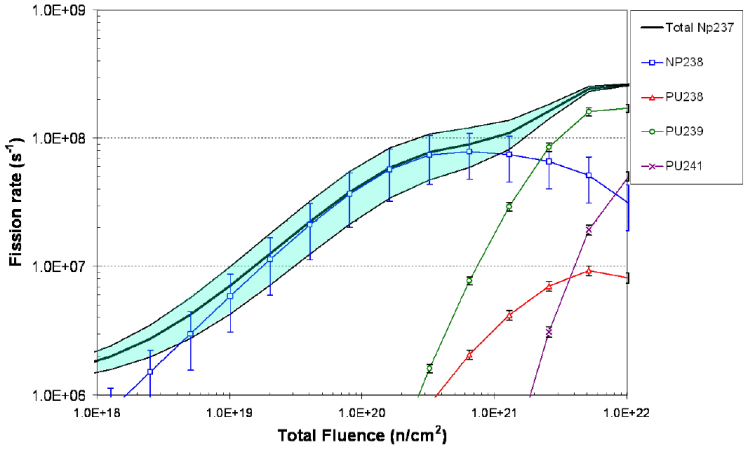
Figure 11. Contribution and error bars (**one standard deviation**) of each isotope in the total fission rate for a deposit of Pu242#2 (see Table I for initial composition) in a typical high flux thermal neutron environment (BR2).



19

PART IV: Relative error in fission rates Np237 in BR2

Figure 12. Total fission rate and error bars (**one standard deviation**) for initially pure Np237 deposit irradiated in a high flux thermal environment (e.g. BR2). Contributions of each isotope to the total fission rate and errors are shown.



5.5/5.6 Decay Heat and Inventory predictions

The need of a database on **Radiation Characterization Benchmark Experiments**:

- **Decay Heat and Inventory Predictions**

Content & Format of evaluations:

1. Detailed description of the experiment:
   - Geometry, materials,… relevant information
2. Evaluation of experimental data
   - Missing data, effects of uncertainties, …
3. Benchmark specifications
   - To provide the data necessary to construct calculational Benchmark-model: Simplifies, Detailed,…
4. Provide results of sample calculations
   - Calculated results,… discrepancies between Benchmark values and calculated values
5. References
6. Appendix A. Typical input listings
7. Appendix B. Supporting information

Procedure:

- Exp. Data:
  FPDH, DH experiments
- PREPRO/NJOY codes
- Activation codes: FISPACT, ACAB, …
- Input data:
  Initial inventory and irradiation history
- Calculate: DH+ΔDH

6. Conclusion

The database on **Radiation Characterization Benchmark Experiments**:

- Quantities not yet included in other Handbooks for "**Radiation Characterization"**
- Pointing out **gaps in experiments/databases** that need to be filled for ND validation
  - IRCBEP benchmarks cover an area not at all covered by ICSBEP, IRPhE or SINBAD because in Radiation Characterization what matter is the "radiation" itself, i.e. the value of the cross sections which allow the description of the radiation
  - How to join efforts: e.g. decay heat for fission events and fusion .vs. SFCOMPO
  - Example of duplicate information:
    - *WP2016-24. Assess the difference of RIKEN neutron spectra compiled in EXFOR E2298 and SINBAD NEA-1552/14 summarized in WP2015-17. N. Outsuka"*
- **Automatize the process of validation**
  - Repository of benchmarks, results… "reproducibility, traceability and transparency"
  - Tools … scripts, updated codes, standard outputs… helping to quickly assess new results
  - Procedures … guidelines to judge validation,…
- **Improve cross-communication** between experts on ND evaluation & experiments