DENIM/UPM activities on:
Nuclear Data Analysis & Processing, Activation-Source Term Calculation and Uncertainty Propagation

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Outline

1. Processing of nuclear data: JEFF/EFF activities
    - 1.1 Activities in JEFF: JEFF-3.1,3.11 and 3.1.2 (JEFF-May-2012)
    - 1.2 Activities in EFF : Photonuclear, DPA and STLs (EFF-Nov-2012)
        - 1.2.1 Processed DPA in multigrous, New IAEA/CRP on dpa
    - 1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

2. Activation and source term calculation
    - 2.1 Description of ACAB code (NEA-1839, DAE-2010 and EFF-Nov-2009)
    - 2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14-JNM-paper), ADS (Annals-EFIT)
    - 2.3 Applications: Burnup Credit (ICNC-2011, ANS-2011, Annals-paper)
    - 2.4 Other work: Fission Chambers (EFF-May-2012 and NIMA-paper)

3. Uncertainty propagation
    - 3.1 Nuclear Data Uncertainties (IAEA-2010)
    - 3.2 Uncertainties in depletion calculation (ANS-2011)
    - 3.3 Examples in: IFE, MFE, IFMIF, ADS (ND-2010)
    - 3.4 Examples in Burnup Credit: PhaseVII (CORDOBA-2009/PHYSOR-2010), Phase-IB (ANS-2011), High Burnup PWR-VandellosII (ICNC-2011)
    - 3.5 Examples in criticality calculations: UAM contributions (UAM5-2011, NCSC2-2011 and UAM6-2012)
    - 3.6 Examples in ESFR: Uncertainty in reactivity coefficients (ND-2013)

4. Summary

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Outline

1. Processing of nuclear data: JEFF/EFF activities
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    - 3.1 Nuclear Data Uncertainties (IAEA-2010)
    - 3.2 Uncertainties in depletion calculation (ANS-2011)
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    - 3.4 Examples in Burnup Credit: PhaseVII (CORDOBA-2009/PHYSOR-2010), Phase-IB (ANS-2011), High Burnup PWR-VandellosII (ICNC-2011)
    - 3.5 Examples in criticality calculations: UAM contributions (UAM5-2011, NCSC2-2011 and UAM6-2012)
    - 3.6 Examples in ESFR: Uncertainty in reactivity coefficients (ND-2013)

4. Summary

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JEFF Meeting, April 25-27, 2012

Processing of the JEFF-3.1.2 Cross Section Library into various formats (ACE, PENDF, GENDF, MATXSR and BOXER) for testing purposes

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1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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JEFF Meeting, April 25-27, 2012

Outline

1. Objectives and planning
   - 1.1 Processing JEFF-3.1.2 in ACE format
   - 1.2 Processing JEFF-3.1.2 to JANIS and BOXER format
   - 1.3 Changes in NJOY99.364
   - 1.4 Updates in JEFF-3.1.2
   - 1.5 Processing TENDL-2011
2. QA procedure
   - 2.1 Warnings & messages in NJOY and PREPRO
   - 2.2 Comparison & visualization
   - 2.3 PREPRO versus NJOY: At low energy, resonances, …
   - 2.4 JEFF-3.1.2 versus ENDF/B-VII.0 - ENDF/B-VII.1
   - 2.5 INTER and BROADR calculation at 293.6K
3. Criticality Validation Suite
   - 3.1 U233, IEU,HEU,LEU and Pu
   - 3.3 Others
4. Summary

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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1.1 Processing JEFF-3.1.2 in ACE

- NJOY99.364 is used to process JEFF-3.1.2 Cross Section Library
- 11 temperatures files: 300K -… - 1800K

Figure 1. NJOY processing sequence for a formatted neutron library

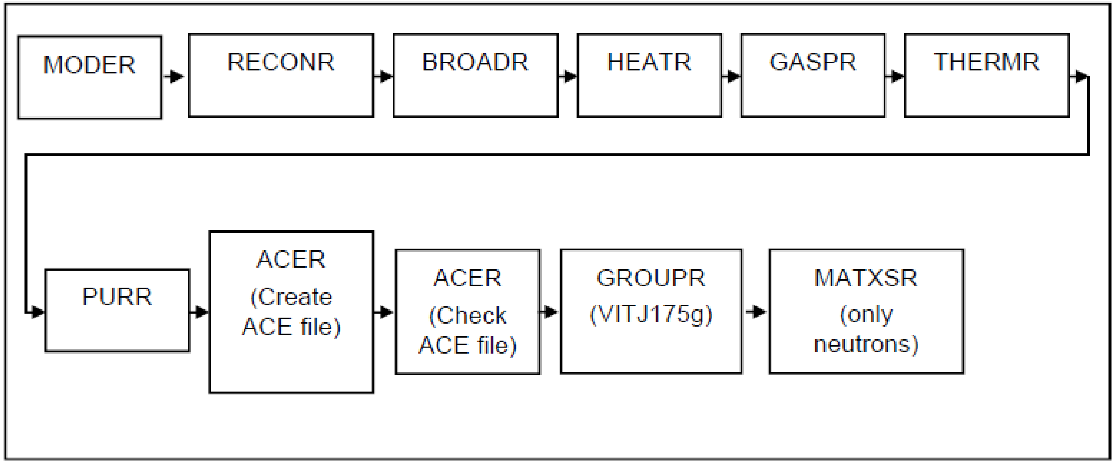

Table 1. Multi-temperature ACE files

#	Temperature (K)	ZAID suffix
1	300	.03c
2	400	.04c
3	500	.05c
4	600	.06c
5	700	.07c
6	800	.08c
7	900	.09c
8	1000	.10c
9	1200	.12c
10	1500	.15c
11	1800	.18c

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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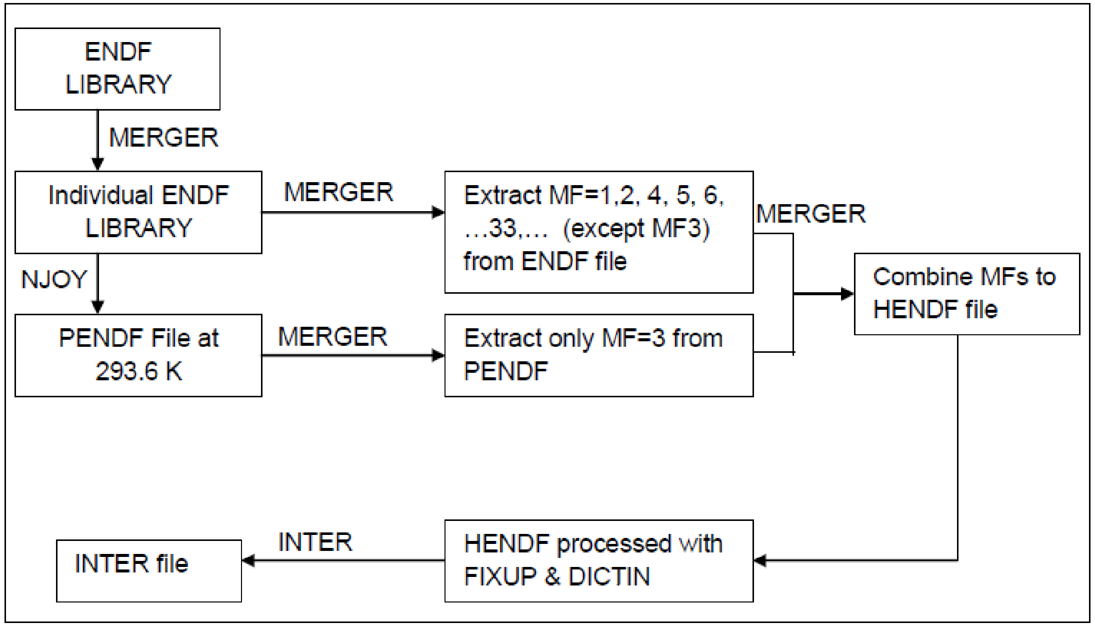
1.2 Processing to JANIS & BOXER

Figure 2. NJOY processing sequence for a JANIS neutron library into BOXER format

MODER → RECONR → BROADR → ERRORR → COVR → VIEWR

Figure 3. Flowchart of processing JANIS library from ENDF tapes



1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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Covariances files: MF31, ..., MF40

Table 4. Processing JEFF-3.1.2 in BOXER format

MAT	Nuclide	MF31	MF32	MF33	MF34	MF35	MF40
131	1-H - 3	-	-	OK	-	-	-
425	4-Be- 9	-	-	OK	-	-	-
600	6-C - 0	-	-	OK	-	-	-
925	9-F - 19	-	-	OK	-	-	-
1425	14-Si- 28	-	-	OK	-	-	-
2225	22-Ti- 46	-	-	OK	-	-	-
2228	22-Ti- 47	-	-	OK	-	-	-
2231	22-Ti- 48	-	-	OK	-	-	-
2234	22-Ti- 49	-	-	OK	-	-	-
2237	22-Ti- 50	-	-	OK	-	-	-
2300	23-V - 0	-	-	OK	-	-	-
2425	24-Cr- 50	-	-	OK	-	-	-
2431	24-Cr- 52	-	-	OK	OK	-	-
2434	24-Cr- 53	-	-	OK	-	-	-
2437	24-Cr- 54	-	-	OK	-	-	-
2525	25-Mn- 55	-	OK	OK	-	-	-

MAT	Nuclide	MF31	MF32	MF33	MF34	MF35	MF40
2625	26-Fe- 54	-	-	OK	-	-	-
2631	26-Fe- 56	-	-	OK	OK	-	-
2634	26-Fe- 57	-	-	OK	-	-	-
2637	26-Fe- 58	-	-	OK	-	-	-
2725	27-Co- 59	-	-	OK	-	-	-
2825	28-Ni- 58	-	-	OK	OK	-	-
2831	28-Ni- 60	-	-	OK	OK	-	-
2834	28-Ni- 61	-	-	OK	-	-	-
2837	28-Ni- 62	-	-	OK	-	-	-
2843	28-Ni- 64	-	-	OK	-	-	-
2925	29-Cu- 63	-	-	OK	-	-	-
2931	29-Cu- 65	-	-	OK	-	-	-
3925	39-Y - 89	-	-	OK	-	-	-
4025	40-Zr- 90	-	-	OK	-	-	-
4125	41- Nb-93	-	-	OK	-	-	OK
7525	75-Re-185	-	-	OK	-	-	-
7531	75-Re-187	-	-	OK	-	-	-
7925	79-Au-197	-	-	OK	-	-	-
9222	92-U -233	OK	OK	OK	OK	OK	-
9228	92-U -235	OK	-	-	-	-	-
9543	95-Am-241	-	-	-	-	-	OK

Isotopes with problems to be processed with NJOY99.364:

- Be9, Si28, Fe54, Nb93, U233

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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Problems processing: U-233

```
moder
1 71
'moder for selected material'
20  9222
0/
moder
1 21
'moder for selected material'
20  9222
0/
reconr
21 24
'PENDF from New EAF-ENDF TENDL2010'/
 9222 /
0.1 0.0 0.20 1.0e-8 9/
0/
broadr
21 24 25
 9222 1 0 1 0.
0.1 /
300.0
0/
errorr
21 25 0 27 0 71/
9222 17 2 1 1/
1 300.0 / mprint temp
 0 33  /Procesa Lib 33 de incertidumbres
9228 18 9228 102/
0/
covr
27 57/
 3 1
'JEFF-3.1.2'/
'Processing BOXER'/
9222 0 0 0 /
covr
27 0 37/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
37 38/
stop
```

NJOY fails due to an error in defining MF32. This problem is solved changing at resonance energies some AJI's now matching with MF2/MT151 (accepted in **JEFF312N9222_0.ASC**)

---message from resprx_rrr_lcomp12---no scattering radius uncertainty

```
7803,7805c7803,7805
< -2.810000+0 2.000000+0 9.795800-4 9.418600-2 3.810800-3 1.357300+0922232151    7
<  1.698200-1 1.000000+0 1.491300-7 6.502000-2 5.587800-2-1.351300-3922232151    8
<  4.401100-1 2.000000+0 1.526300-6 9.144900-4 2.317600-1 1.106800-1922232151    9
---
>  2.810000+0 3.000000+0 9.795800 4 9.418600 2 3.810800 3 1.357300+0922232151    7
>  1.698170-1 3.000000+0 1.491300-7 6.502000-2 5.587800-2-1.351300-3922232151    8
>  4.401140-1 2.000000+0 1.526300-6 9.144900-4 2.317600-1 1.106800-1922232151    9
...
```

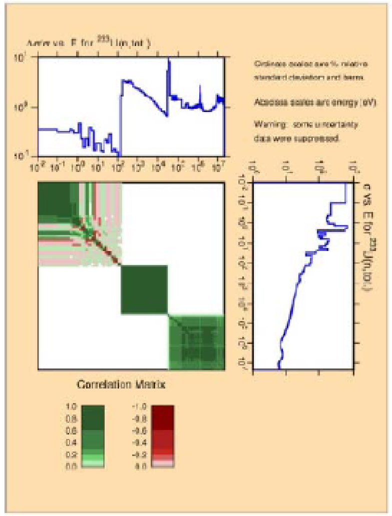

Figure 12. Processing MF33- ^{233}U

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2. QA procedure

2.1 Comparison & visualization

2.2 Warnings & messages in NJOY and PREPRO

2.3 PREPRO versus NJOY: At low energy, resonances, …

2.4 JEFF-3.1.2 versus ENDF/B-VII.0 - ENDF/B-VII.1

2.5 INTER and BROADR calculation at 293.6K

2.1 QA procedure: comparison & visualization

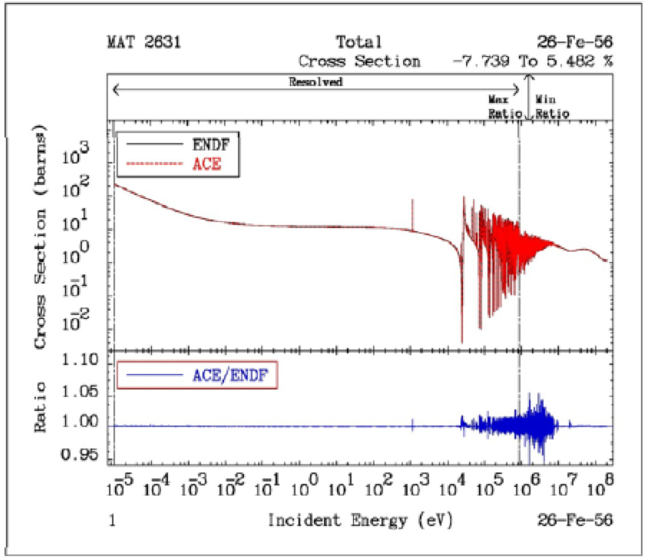

Figure 14. Example of Q&A with ACELST code Fe-56

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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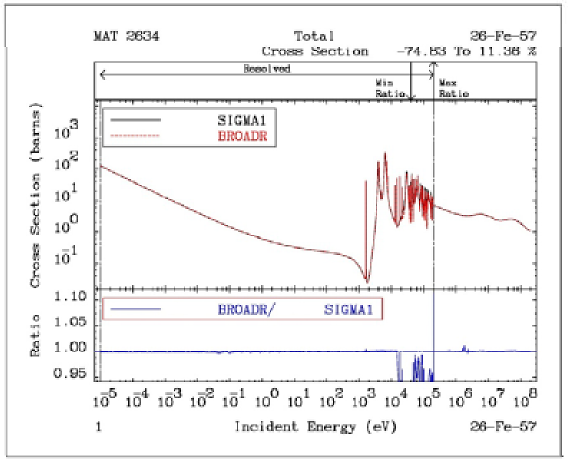
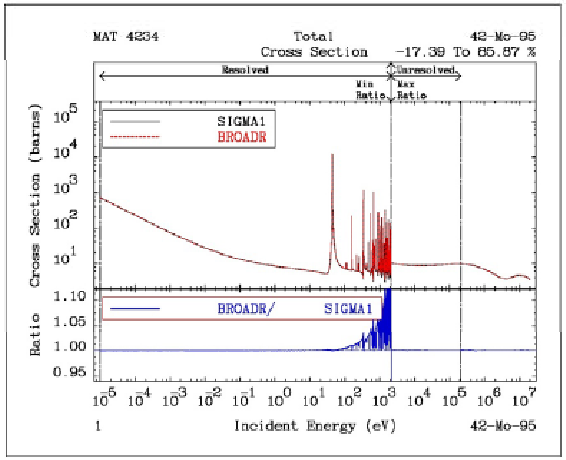
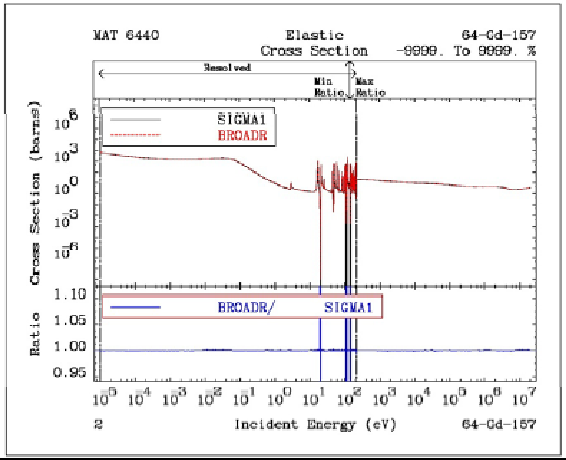
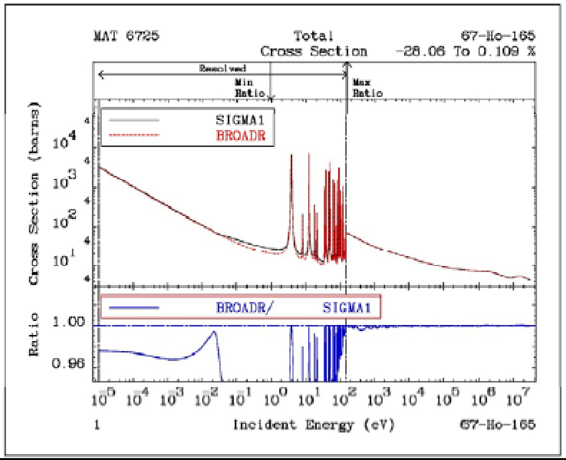
PREPRO vs NJOY: Resonances









1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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2.4 JEFF-3.1.2 vs ENDF/B-VII.0-VII.1

Figure 17. Total cross-section Hf-176

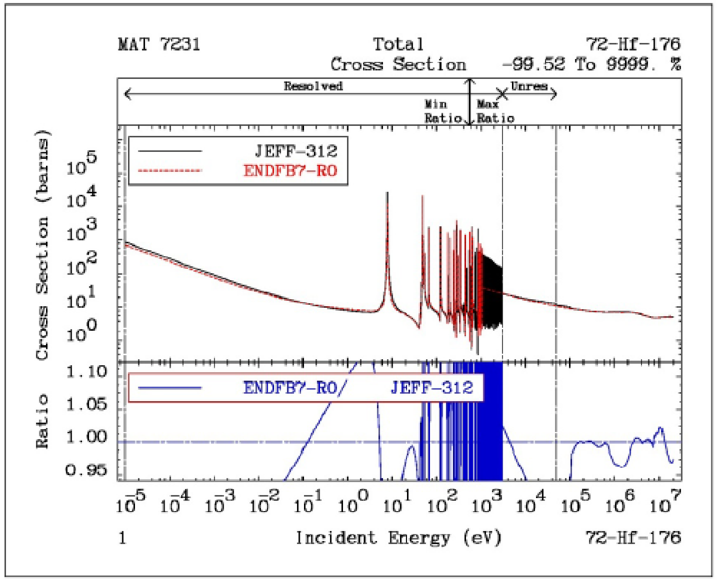
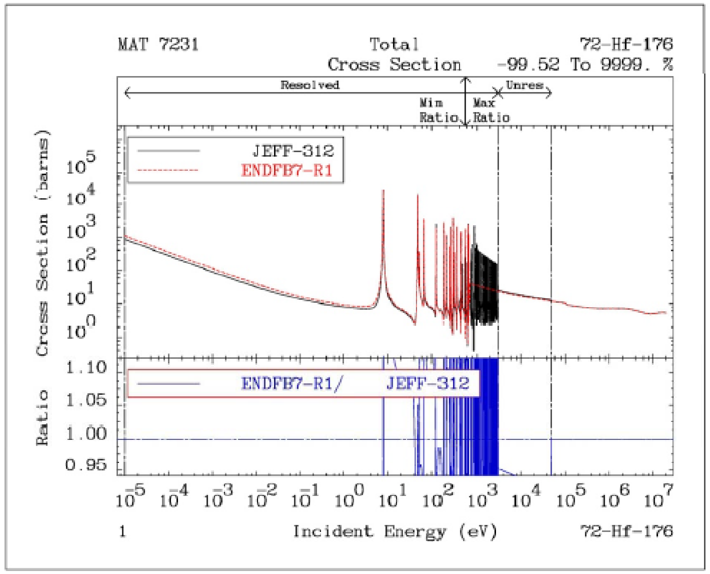


Figure 18. Total cross-section Hf-176



1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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2.5 INTER calculation at 293.6K

Material number (MAT) = 721760 NAME= hf176

LIBRARY	Z	A	LISO	LFS	MT	Reaction	Sig(2200)	Sig(Ezero)	Avg-Sigma	G-fact	Res Integ	Sig(Fiss)	Sig(E14)
EAF-2007	72	176	0		1	Total	1.40636E+01	1.40536E+01	1.4093E+01	1.00285	6.09825E+02	1.54606E-01	1.96095E+00
ENDFB-6.8	72	176	0		1	Total	2.04851E+01	2.04753E+01	2.1353E+01	1.04316	7.70696E+02	7.02399E+00	5.30000E+00
ENDFB-7.0	72	176	0		1	Total	2.04851E+01	2.04753E+01	2.1353E+01	1.04316	7.70696E+02	7.02399E+00	5.30000E+00
ENDFB-7.1	72	176	0		1	Total	2.69430E+01	2.69278E+01	2.7685E+01	1.02832	1.11627E+03	7.13610E+00	5.37211E+00
JEF-2.2	72	176	0		1	Total	1.85566E+01	1.85466E+01	1.9159E+01	1.03325	9.71128E+02	6.98886E+00	5.67229E+00
JEFF-3.0	72	176	0		1	Total	2.90479E+01	2.90313E+01	2.9811E+01	1.02704	1.42899E+03	7.22047E+00	5.37211E+00
JEFF-3.0A	72	176	0		1	Total	1.40636E+01	1.40537E+01	1.4093E+01	1.00283	6.10193E+02	9.53312E-02	1.96144E+00
JENDL-3.3	72	176	0		1	Total	2.90479E+01	2.90313E+01	2.9811E+01	1.02704	1.42899E+03	7.14147E+00	5.37211E+00
TENDL-2008	72	176	0		1	Total	2.88987E+01	2.88820E+01	2.9623E+01	1.02585	1.12074E+03	7.04831E+00	5.37230E+00
TENDL-2011	72	176	0		1	Total	2.88980E+01	2.88817E+01	2.9621E+01	1.02578	1.13440E+03	7.15742E+00	5.30539E+00
JEFF-3.1.1	72	176	0		1	Total	2.68571E+01	2.68419E+01	2.7596E+01	1.02828	1.12113E+03	7.14147E+00	5.37211E+00
JEFF-3.1.2	72	176	0		1	Total	2.21498E+01	2.21378E+01	2.2845E+01	1.03215	1.04242E+03	7.14086E+00	5.37211E+00

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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2.7 BROADR calculation at 293.6K

JEFF-3.1.2 has been processed at 293.6 K (.0253 eV), **BROADR computes**:

- fission cross section at thermal
- fission nu-bar at thermal
- capture cross section at thermal
- thermal Maxwellian fission integral
- thermal Maxwellian capture integral
- fission g-factor (deviation from 1/*v*)
- capture g-factor
- thermal alpha integral
- thermal eta integral
- thermal K1 integral
- fission resonance integral
- capture resonance integral

Material number (MAT) = 721760 NAME= hf176

LIBRARY	the fis xs	the fis nb	the cap xs	the cap int	cap res int	the fis int	the fis g-f	the alp int	...
EAF-2007	0.00000E+00	0.00000E+00	1.40640E+01	1.24990E+01	6.10530E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
ENDFB-6.8	0.00000E+00	0.00000E+00	1.37630E+01	1.22170E+01	4.00720E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
ENDFB-7.0	0.00000E+00	0.00000E+00	1.37630E+01	1.22170E+01	4.00720E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
ENDFB-7.1	0.00000E+00	0.00000E+00	2.13840E+01	1.89990E+01	6.94410E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JEF-2.2	0.00000E+00	0.00000E+00	1.40550E+01	1.24920E+01	6.14270E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JEFF-3.0	0.00000E+00	0.00000E+00	2.34900E+01	2.08860E+01	8.93150E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JEFF-3.0A	0.00000E+00	0.00000E+00	1.40640E+01	1.24990E+01	6.10670E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JENDL-3.3	0.00000E+00	0.00000E+00	2.34900E+01	2.08860E+01	8.93150E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
TENDL-2008	0.00000E+00	0.00000E+00	2.34770E+01	2.08550E+01	7.12520E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
TENDL-2011	0.00000E+00	0.00000E+00	2.34760E+01	2.08530E+01	7.13690E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JEFF-3.1.1	0.00000E+00	0.00000E+00	2.13280E+01	1.89490E+01	6.94460E+02	0.00000E+00	0.00000E+00	0.00000E+00	...
JEFF-3.1.2	0.00000E+00	0.00000E+00	1.68500E+01	1.49650E+01	6.33610E+02	0.00000E+00	0.00000E+00	0.00000E+00	...

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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3. Criticality Validation Suite

- An expanded Criticality Validation Suite, taken from Integral Benchmark Experiments, ICSBEP for Criticality Safety.
- Presented by *R.D. Mosteller, F.B. Brown and B.C. Kiedrowski* in ICNC2011 to test ENDF/B-VII.1β3 containing **119 cases** **[LA-UR-11-04170]** for a variety of fuels. A comparison with **[NEA/JEFF-3.1.1]** is also performed in this work:
  - ✓ ^{233}U : 18
  - ✓ Highly enriched uranium (HEU) : 40
  - ✓ Intermediate-enriched uranium (IEU): 17
  - ✓ Low-enriched uranium (LEU) : 8
  - ✓ Plutonium : 36
- For each type of fuel, there are cases with a variety of:
  - ✓ Moderators
  - ✓ Reflectors
  - ✓ Spectra
  - ✓ Geometries
- In addition, 4 cases also included in ICSBEP are used for testing purposes:
  - ✓ Np237
  - ✓ Heavy-Water solutions
  - ✓ Very thermal Pu solution
  - ✓ Unmoderated ZEUS benchmark

1. Processing of nuclear data: JEFF/EFF activities

1.1 Activities in JEFF: JEFF-3.1, 3.11 and 3.1.2 (JEFF-May-2012)

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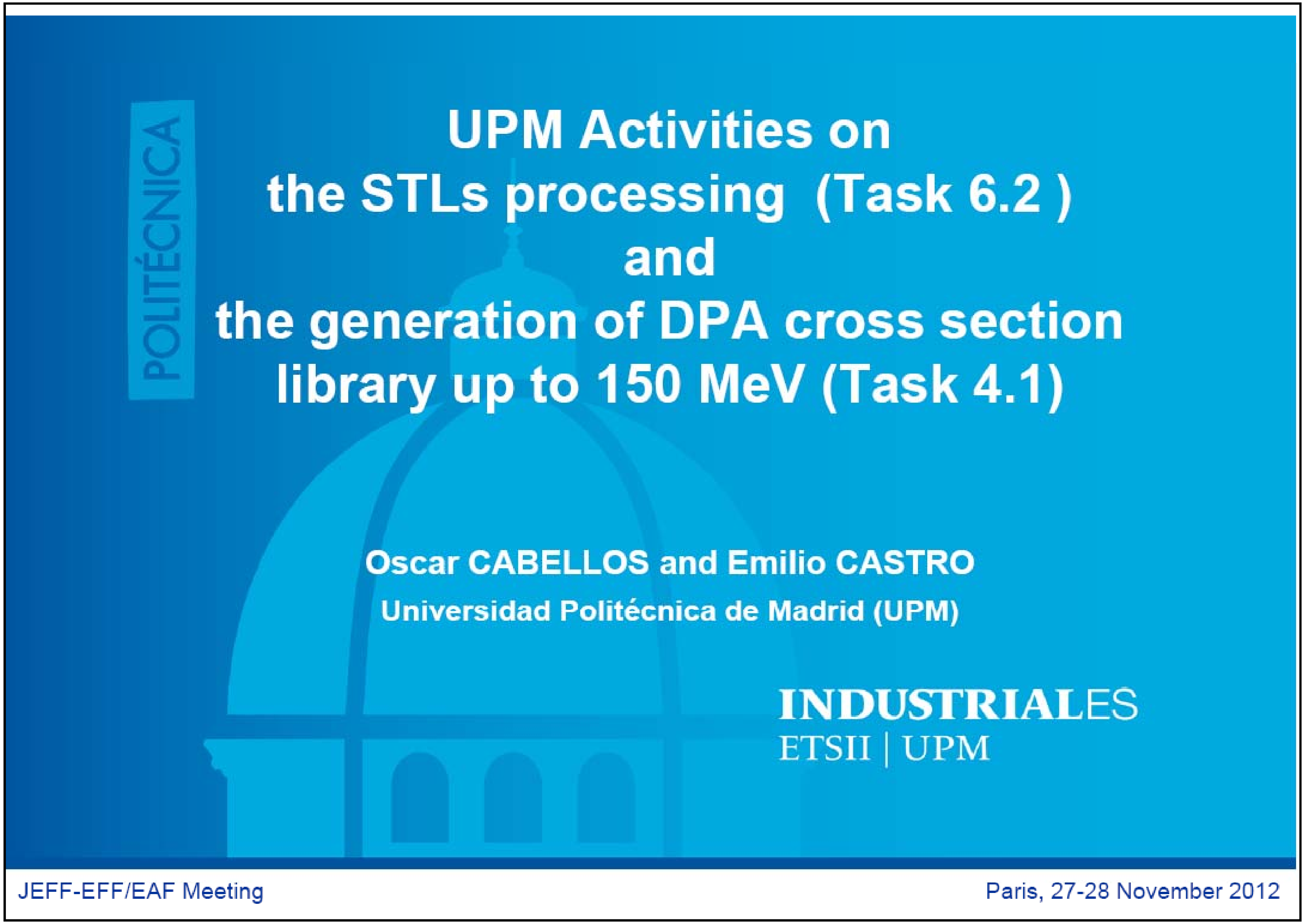
^{233}U Benchmarks

					keff				
						LA-UR-11-04170 & ICNC2011, R.D. Mosteller		This work	
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII.0[*]	ENDF/B-VII.1β3[*]	JEFF-3.1.2 300K	JEFF-3.1.2 293.6K
Fast	Metal	Spheres	Unreflected	u233-met-fast-001	1.0000±0.0010	0.9996±0.0003	0.9995±0.0003	1.00423±0.00025	1.00450±0.00025
			HEU	u233-met-fast-002-CASE_1	1.0000±0.0010	0.9986±0.0003	0.9990±0.0003	1.00251±0.00026	1.00257±0.00027
				u233-met-fast-002-CASE_2	1.0000±0.0011	1.0002±0.0003	1.0006±0.0003	1.00404±0.00026	1.00322±0.00026
			Normal Uranium	u233-met-fast-003-CASE_1	1.0000±0.0010	0.9990±0.0003	0.9996±0.0003	1.00485±0.00026	1.00512±0.00028
				u233-met-fast-003-CASE_2	1.0000±0.0010	0.9993±0.0003	1.0001±0.0003	1.00481±0.00029	1.00493±0.00028
				u233-met-fast-006	1.0000±0.0014	0.9987±0.0003	0.9995±0.0003	1.00541±0.00031	1.00576±0.00031
			Tungsten	u233-met-fast-004-CASE_1	1.0000±0.0007	0.9987±0.0003	1.0049±0.0003	1.00521±0.00029	1.00547±0.00027
				u233-met-fast-004-CASE_2	1.0000±0.0008	0.9954±0.0003	1.0052±0.0003	1.00413±0.00027	1.00372±0.00027
			Beryllium	u-233-met-fast-005-CASE_1	1.0000±0.0030	0.9963±0.0003	0.9941±0.0003	1.00043±0.00027	Beo STL
				u-233-met-fast-005-CASE_2	1.0000±0.0030	0.9956±0.0003	0.9924±0.0003	1.00032±0.00030	Beo STL
Intermediate	Solution	Sphere	Beryllium	u233-sol-inter-001-case1	1.0000±0.0083	-	0.9848±0.0005	0.98412±0.00049	0.98389±0.00048
Thermal	UO2+ZrO2	Lattice	Water	u233-comp-therm-001-case3	1.0000±0.0024	-	1.0045±0.0005	0.99739±0.00047	0.99759±0.00048
	Solution	Sphere	Unreflected	u233-sol-therm-001-case1	1.0000±0.0031	-	1.0015±0.0003	0.99892±0.00026	0.99866±0.00026
				u233-sol-therm-001-case2	1.0000±0.0033	-	1.0011±0.0003	0.99832±0.00026	0.99881±0.00024
				u233-sol-therm-001-case3	1.0000±0.0033	-	1.0009±0.0009	0.99863±0.00025	0.99829±0.00025
				u233-sol-therm-001-case4	1.0000±0.0033	-	1.0019±0.0003	0.99873±0.00026	0.99793±0.00026
				u233-sol-therm-001-case5	1.0000±0.0033	-	0.9996±0.0003	0.99736±0.00027	0.99798±0.00027
				u233-sol-therm-008	1.0000±0.0029	-	1.0012±0.0002	0.99807±0.00018	0.99810±0.00017

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$



POLITÉCNICA
UPM Activities on
the STLs processing (Task 6.2)
and
the generation of DPA cross section
library up to 150 MeV (Task 4.1)
Oscar CABELLOS and Emilio CASTRO
Universidad Politécnica de Madrid (UPM)
INDUSTRIALES
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JEFF-EFF/EAF Meeting
Paris, 27-28 November 2012

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Task 6.2 : Photonuclear Libraries

Recent Photonuclear Libraries

Libraries	IAEA	JENDL/PD-2004	ENDF/B-VII.1	TENDL-2009 TENDL-2011
Energy	< 140 MeV	< 140 MeV	< 150 MeV *20-30 MeV	200 MeV
Materials	164	68	163	^{6}Li – ^{281}Ds
Evaluation Methods	GNASH + statistic	Better (γ,abs) Exp Data	IAEA Revision Exp. Bremsstr.	TALYS
Others		He, Li, B, F, P, Hg y Gd	Actinides	Isomeric States

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Task 6.2 : A comparison ...

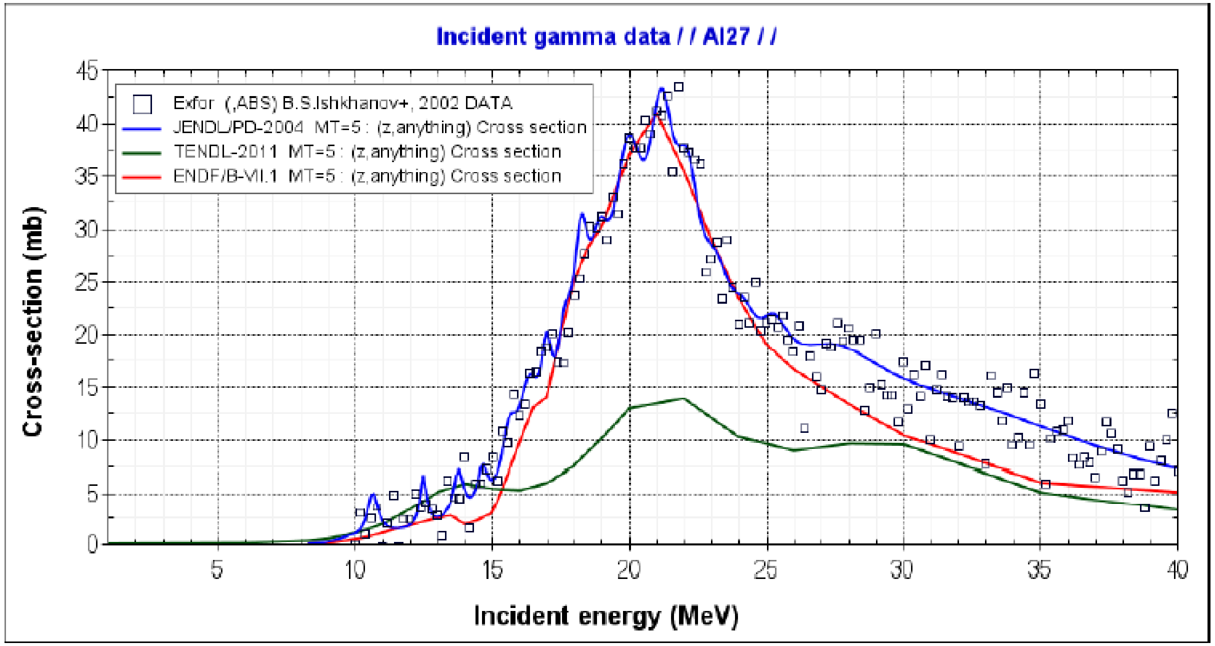

Figure. A comparison of total gamma cross section for Al27.
JEFF-3.1.1, ENDF/B_VII.1 and JENDL-PD. Exfor Data: Ishkhanov 2002

Exfor data: Moscow State Uiversity. Nuclear Physics Intitute. Ishkhanov *et al.* 2002
Source: Quasi-monoenergetic photons, Annihilation radiation.

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Task 6.2 : Processing with NJOY...

```
moder / Extract/convert
photonuclear data
1 41
'26-Fe-54 from ENDF/B-VII'/
40 2625
0/
moder / Extract/convert
photonuclear data
1 42
'26-Fe-54 from ENDF/B-VII'/
40 2625
0/
acer / Prepare ACE files
41 42 0 27 28
5/
'26-Fe-54 photo-nuclear'/
2625/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
stop
```

Figure. NJOY Input to process Photonuclear Evaluated Files in ACE format

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Task 6.2 : Application with MCNPX

Material	Electron beam	Neutron Yield per 10^6 Electrons					
Target	Energy	Data Exp. B&G **	COG*	MCNPX IAEA*	MCNPX ENDF/B-VII.1 *This Work*	MCNPX JENDL PD-2004 *This Work*	MCNPX TENDL-2011 *This Work*
Aluminium	22.2 MeV	*46 ± 7*	*37 ± 1*	*35*	**37**	**37**	**23**
Aluminium	28.3 MeV	*210 ± 32*	*162 ± 1*	*158*	**170**	**170**	**130**
Aluminium	34.3 MeV	*430 ± 65*	*332 ± 2*	*329*	**330**	**330**	**250**

*Ref. Photonuclear Benchmarks with a Comparison of COG and MCNPX. David P. Heinrichs and Edward M. Lent. Cross Section Evaluation Working Group (CSEWG) at the Meeting held at Brookhaven National Laboratory, November 4 - 6, 2003.

**Experiment: W. C. Barber and W. D. George, “Neutron Yields from Targets Bombarded by Electrons”, Physical Review: 116 (6) 1551 – 1559, December 15, 1959

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DPA Processing with NJOY.
Task 4.1 : Approximations above 20 MeV ?

- Approximation: JEFF-3.1.1 with MT5-MT6 taken from ENDF/B-VII.1

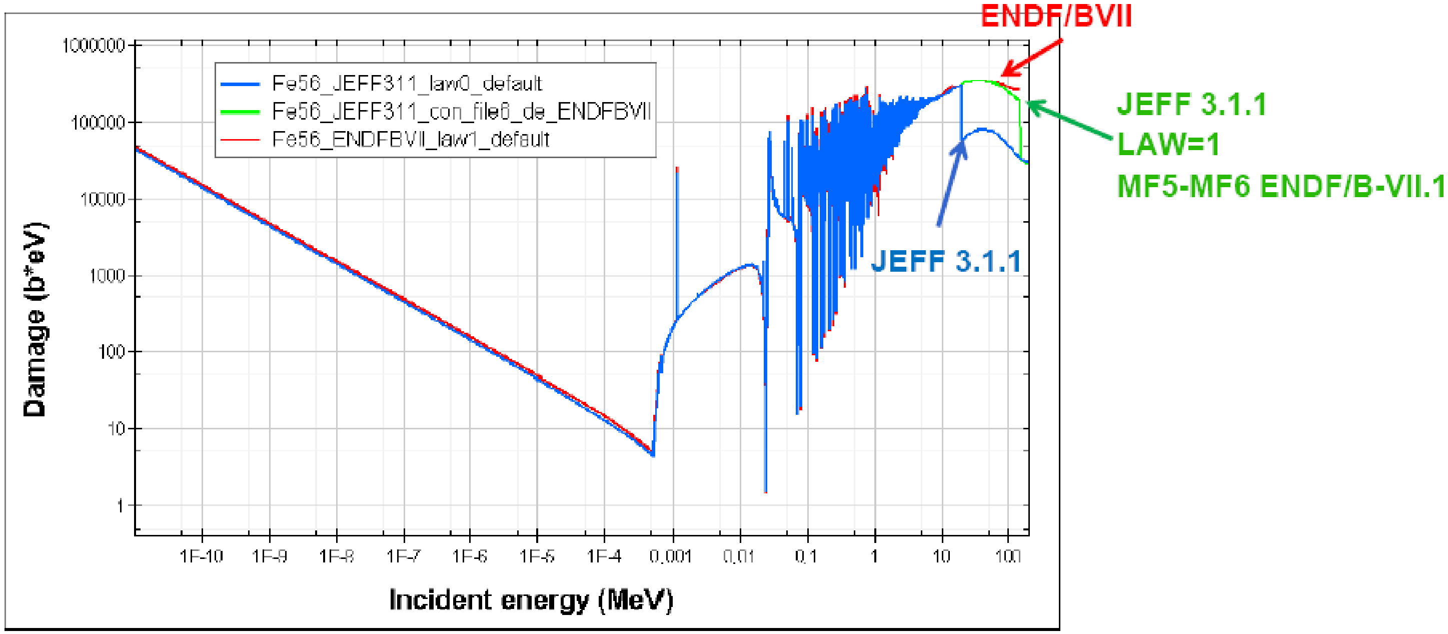

Figure. A comparison of Damage Energy Cross Section for Fe56.
Updated JEFF-3.1.1 with MT5 and MT6 taken from ENDF/B-VII.1

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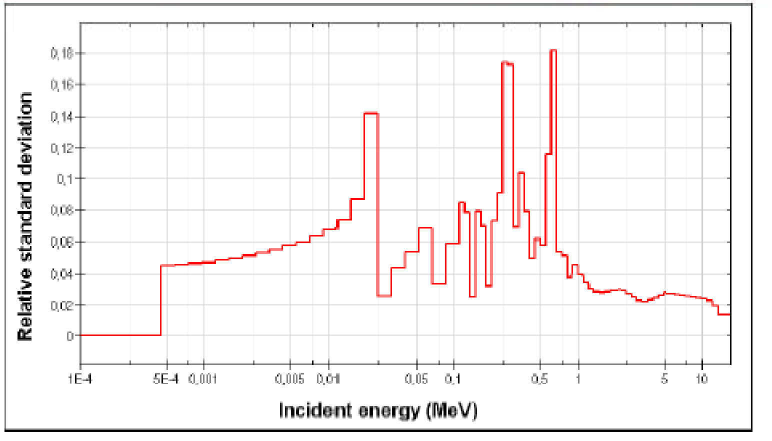
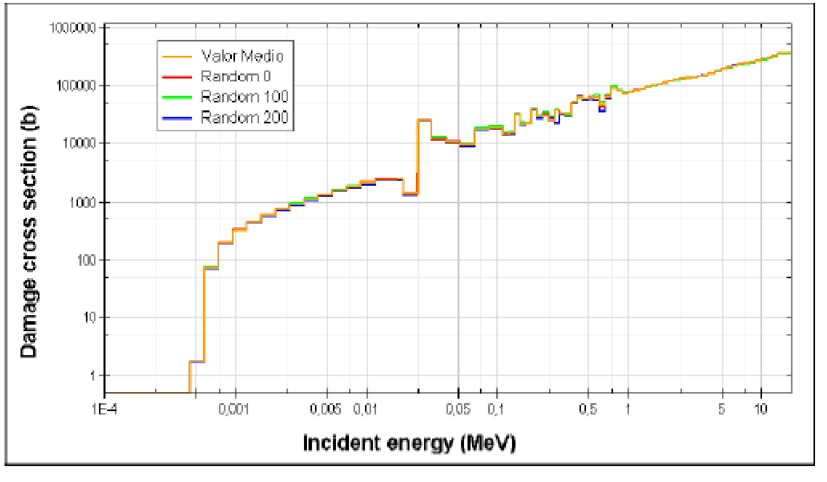
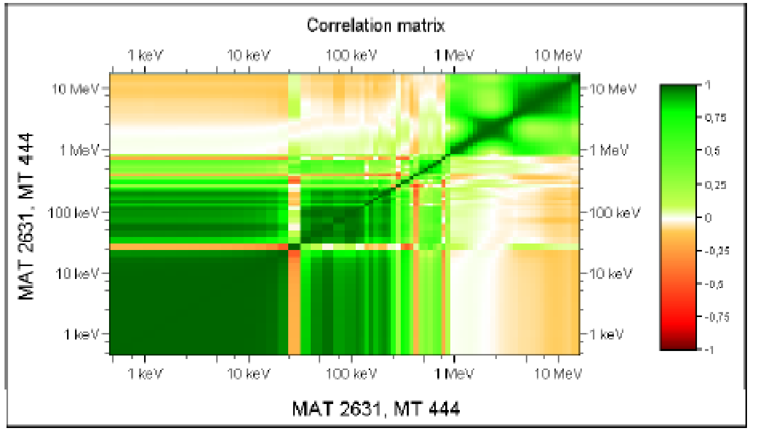
Task 4.1 : What about uncertainties?

Based on Total Monte Carlo methodology

- TENDL2011: 380 ENDF files
- Processing with NJOY/GROUPR







1. Processing of nuclear data: JEFF/EFF activities

1.2 Activities in EFF : Photonuclear, DPA and STLs (EFF-Nov-2012)

Processed DPA library in multigrous

Home | About Us | Work Areas | Data Bank | Publications | Delegates' Area

NEA
Nuclear Energy Agency

NEA search engine Go

Data Bank > Nuclear Data Services

Nuclear application data (processed libraries and tools)

In order to support the distribution and best use of the various evaluated nuclear data libraries, the NEA promotes the exchange of information on processed libraries, pre-processing and processing codes. The NEA also provides a framework for the processing of evaluated nuclear data through its nuclear data services. New libraries are always being sought and added to this listing. Available application data libraries are listed below, along with links to useful processing tools.

Workshop on Processing tools for evaluated nuclear data libraries

NEA Offices, France on the 18 November 2008

Tools for the checking and processing of nuclear data

Several checking and processing and viewing tools exist, some of which are listed below:

- PREPRO
- ENDF checking codes
- NJOY
- NJOY User Group Meeting, 26 November 2007

ENDF/B-VII.0 data processed with NJOY-99.259 for radiation damage calculations

(Including extensions to important reactions for activation.)
Date: December 2007.
The library was prepared by Oscar Cabellos (UPM, Spain).

http://www.oecd-nea.org/dbdata/process/

New IAEA/CRP on dpa

IAEA Coordinated Research Project (CRP) "Primary Radiation Cross Sections" was approved in Dec. 2012 (F44003, see http://www-crp.iaea.org/html/rifa-show-approvedcrp.asp).

1. **Asses the accuracy and completeness of current Nuclear Data that are used to calculate material radiation damaging.**

2. Calculation/evaluation of number of Primary Radiation Defects (PRD), i.e. Frenkel Pairs (FPs) and in-cascade clusters, survived after cascade athermal quenching (time span up to 10ps – 1 ns) - being expressed as ratio to dpa-NRT is also often called as damage or cascade efficiency.

3. Incorporation of damage efficiency in nuclear data processing and generation database of damage energy and atom displacement cross sections for PRD.

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Task 6.2 : STLs

Processing of all Thermal Scattering Libraries in multigroups and ACE format using NJOY.

- Introduction to Thermal Scattering Libraries
- TSL in ENDF-6 format
- State of the Art
- Processing with NJOY
- Graphics

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State of the Art: Temperatures

Isotope	Compound	ENDF/B-VI.8 and JENDL-4.0. 20 materials	ENDF/B-VII.0 and ENDF/B-VII.1 20 and 21 mats.	INDL-TSL 11 materials	JEFF 3.1.X 9 materials
H	H2O Problems processing all libraries	296, 350, 400, 450, 500, 600, 800, 1000	293.6, 350, 400, 450, 500, 550, 600, 650, 800	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000	293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6, 647.2, 800, 1000
H	Para-H	20	20	14, 16, 20.38	-
H	Ortho-H	20	20	14, 16, 20.38	-
H	HZr	296, 400, 500, 600, 700, 800, 1000, 1200 Without secondary scatterer.	296, 400, 500, 600, 700, 800, 1000, 1200 Without secondary scatterer.	293.6, 400, 500, 600, 700, 800, 1000, 1200 With secondary scatterer.	293.6, 400, 500, 600, 700, 800, 1000, 1200 With secondary scatterer.
H	CaH2	-	-	-	296, 400, 500, 600, 700, 800, 1000, 1200
H	TiH2	-	-	293.6, 400, 500, 600, 700, 800, 1000, 1200	-

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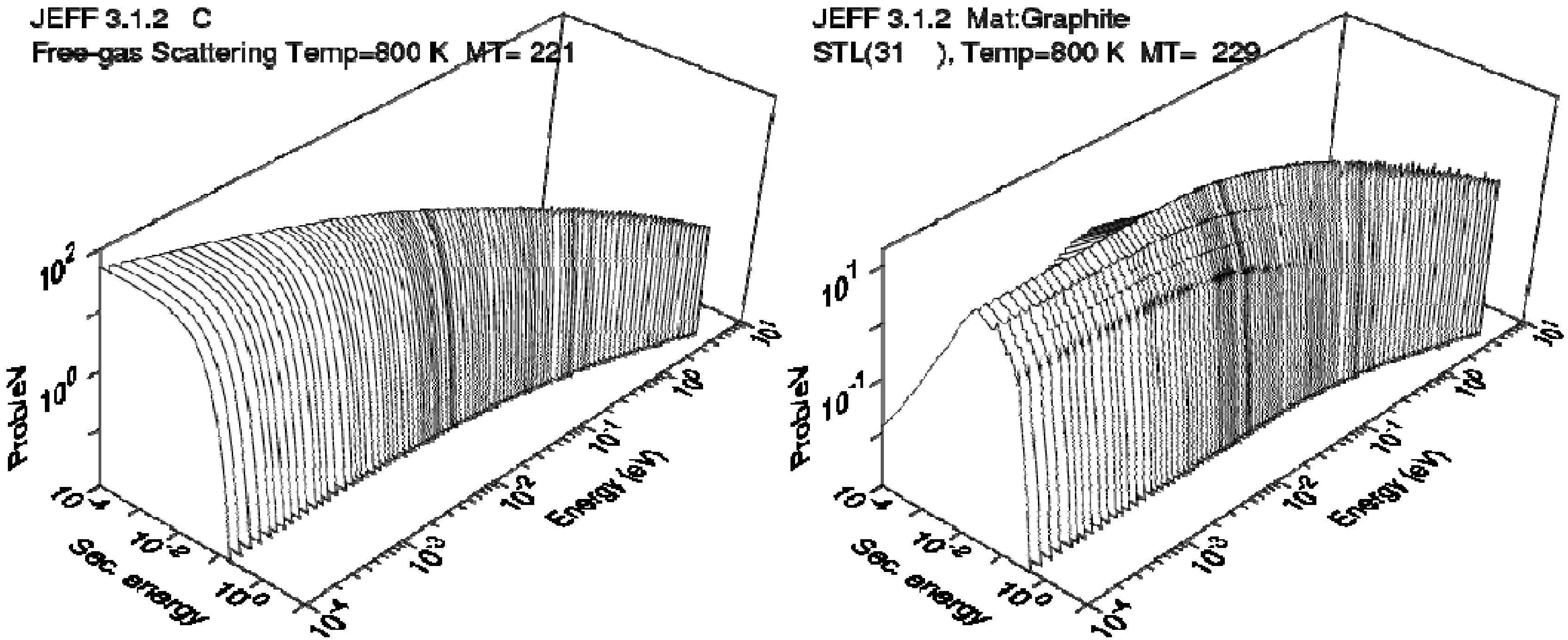
Graphics

While processing, graphics for all materials have been generated for all available temperatures using the modules plotr and viewr of NJOY.

There are two kind of graphics: Free gas scattering and Bound scattering



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Calculations of Fission Pulse Neutron Emission:

A comparison between JEFF-3.1.1. and ENDF/B-VII.1

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CIEMAT, Spain

JEFF Measurement, Evaluation, Processing and Benchmarking
April 25-27, 2012
1

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1. Objective of this work

- To test the present status of Evaluated **Decay Data** and **Fission Yield** data libraries to predict:
  - the neutron emission rate
  - average neutron energy and neutron delayed spectra
- A comparison of these values with ***Keepin* formula** with values taken from Evaluated XS Data Libraries (MT455)
- Calculations performed with **JEFF-3.1.1 and ENDF/B-VII.1**

  JEFF 3.1.1 : 241 βn-emitter, 18 β2n-emitter and only 4 β3n-emitters

  ENDF/B-VII.1 : 390 βn-emitter, 111 β2n-emitter, 14 β3n-emitter and 2 β4n-emitter
- Prediction of "**uncertainties**" due to the current uncertainties in these Nuclear Data Libraries
- Calculations are performed with **ACAB code** (NEA-1839 ACAB-2008)

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2. Total delayed neutron emission

- **The total delayed neutron emission per fission** can be calculated as follow: $\overline{\nu}_d = \sum_i P_{ni} \cdot c_i$

  where:

  c_i is the cumulative yields of isotope-i, taken from *"Evaluated Fission Yield Data Library"*

  P_{ni} is the probability of a nuclide-i emitting a neutron as a result of a beta decay *"Evaluated Fission Decay Data Library"*

- The uncertainty in the calculated $\overline{\nu}_d$ can be estimated assuming c_i and P_{ni} are independent:

$$\mathrm{var}(\overline{\nu}_d) = \sum_i P^2_{ni} \cdot \mathrm{var}(c_i) + \mathrm{var}(P_{ni}) \cdot c^2_i$$

Table 1. Average delayed neutron yields following a **single 14 MeV fission**

Nuclide	Energy	*Calculated JEFF-3.1.1 neutron per 100 fission	My work with JEFF-3.1.1		My work with ENDF/B-VII.1	
^{232}Th	14 MeV	3.05 ± 0.03	**3.04**	**± 0.21**	**5.67**	**± 0.31**
^{233}U	14 MeV	0.55 ± 0.01	**0.56**	**± 0.06**	**0.71**	**± 0.10**
^{235}U	14 MeV	0.93 ± 0.02	**0.93**	**± 0.07**	**1.26**	**± 0.14**
^{238}U	14 MeV	2.36 ± 0.03	**2.36**	**± 0.10**	**2.74**	**± 0.21**

* *M.A. Kellet, O. Bersillon, R.W. Mills, The JEFF-3.1/3.1.1 radioactive decay data and fission yields sub-libraries, JEFF Report 20, NEA/OECD, 2009*

Validation of Uncertainty Methodologies: "Checking or comparing different uncertainty methods"

1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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2.1 Importance of nuclides

Table 2. Example: Thermal fission of ^{235}U of JEFF-3.1.1. Decay data relative error (r.e. in %) of P_{ni} and C_{ni}. Nuclides sorted by relative importance of total neutron emission.

ANDES. WP1
Measurements for advanced reactor systems.

- *Subtask 1.4.b. β-delayed neutron emission probabilities of 88Br, 94Rb, 95Rb and 137I*

#	Nuclide	P_{ni}	rel.error (P_{ni}) in %	c_i	rel.errorr (c_i) in %		$\frac{P_{ni}\cdot c_i}{\bar{V}_d}*100$	$\frac{\mathrm{var}(P_{ni}\cdot c_i)}{\mathrm{var}(\bar{V}_d)}*100$
1	I-137	6.50E-02	6.15	3.57E-02	7.14		15.81	7.69
2	Br-89	1.41E-01	2.84	1.36E-02	17.58		13.04	18.67
3	Rb-94	1.01E-01	1.98	1.50E-02	21.45		10.29	17.01
4	Br-88	6.70E-02	2.99	1.82E-02	8.71		8.29	2.02
5	Br-90	2.46E-01	2.85	4.87E-03	31.55		8.15	23.10
6	I-138	5.30E-02	5.66	1.47E-02	22.51		5.31	5.25
7	Y-98m	3.44E-02	27.62	1.97E-02	13.45		4.63	6.99
8	I-139	9.80E-02	4.08	5.98E-03	31.04		3.99	5.41
9	Rb-95	8.60E-02	2.33	6.58E-03	30.19		3.86	4.72
10	Br-87	2.51E-02	3.19	2.14E-02	2.32		3.65	0.07
11	Rb-93	1.40E-02	5.71	3.54E-02	7.17		3.38	0.33
12	Y-99	1.70E-02	23.53	1.88E-02	17.37		2.18	1.41
13	As-85	2.20E-01	13.64	1.43E-03	29.29		2.14	1.66
14	Br-91	2.00E-01	10.00	1.52E-03	34.38		2.07	1.89
15	Sb-135	1.57E-01	7.64	1.79E-03	33.93		1.91	1.53
16	Cs-143	1.64E-02	-	1.65E-02	18.77		1.84	0.41
17	As-86	3.30E-01	-	4.45E-04	34.90		1.00	0.42
18	Rb-96	1.34E-01	2.99	1.01E-03	25.93		0.92	0.20
19	Cs-145	1.43E-01	5.59	9.02E-04	34.38		0.88	0.32
20	I-140	9.30E-02	-	1.21E-03	34.91		0.76	0.25
21	Cs-144	3.20E-02	-	3.17E-03	24.46		0.69	0.10
22	Te-137	1.50E-02	-	4.81E-03	31.00		0.49	0.08
23	Br-92	3.31E-01	-	2.00E-04	34.74		0.45	0.09
24	Rb-97	2.51E-01	3.19	2.50E-04	35.15		0.43	0.08
25	Te-138	6.30E-02	-	9.40E-04	36.68		0.40	0.08
...	....	...	...	...	...		...	..
144	Ru-119	4.36E-02	1.01	3.91E-11	38.85		0.00	0.00

1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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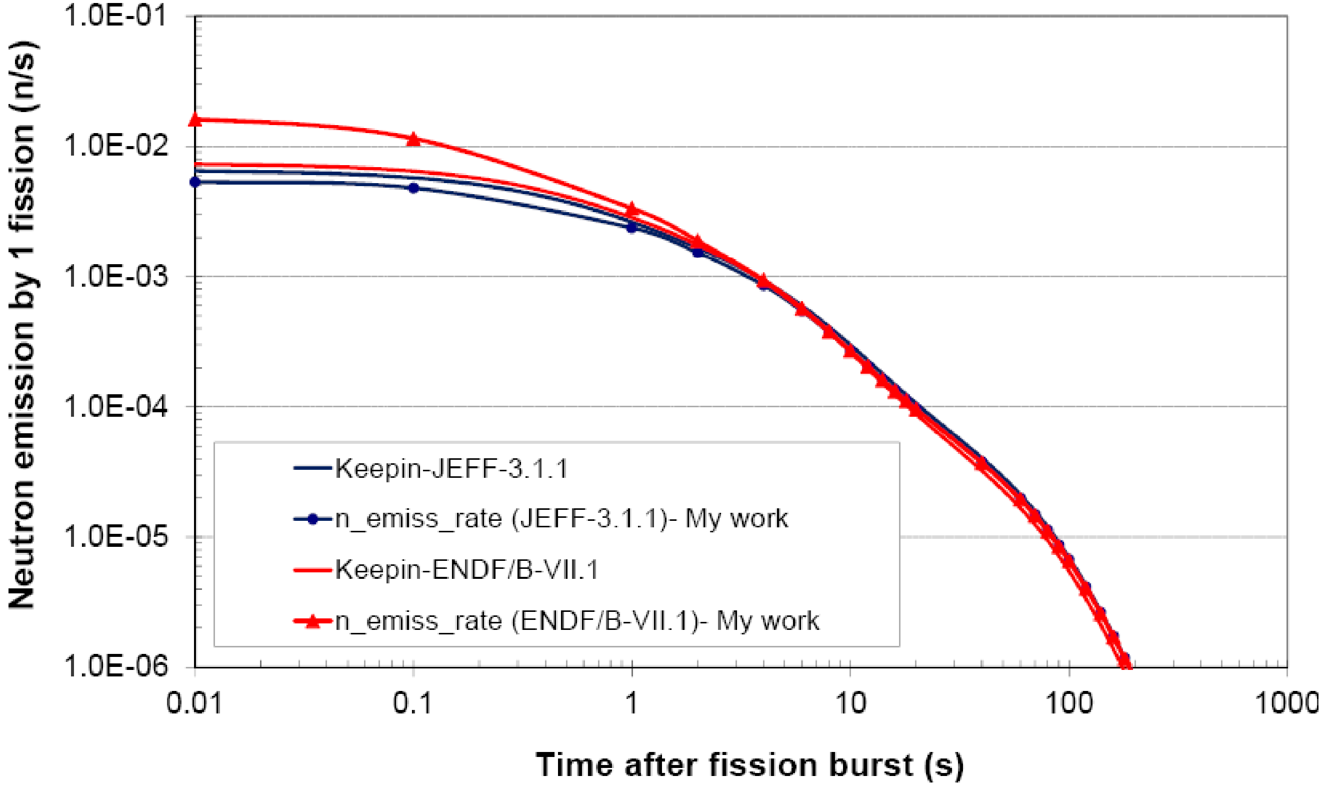
3.1 $n_{emit}(t)$: "Keepin 6/8-g formula"

- For ENDF/B-VII.1, at t=0s diff. ~128% between Keepin formula and Decay&FY Data

Nemission rate calculated with Decay&FY Data overestimates Keepin formula!!

Figure 1. Comparison of delayed neutron emission rate, $n_{emit}(t)$, calculated using Keepin 6/8-group formula and Decay&FY Data



1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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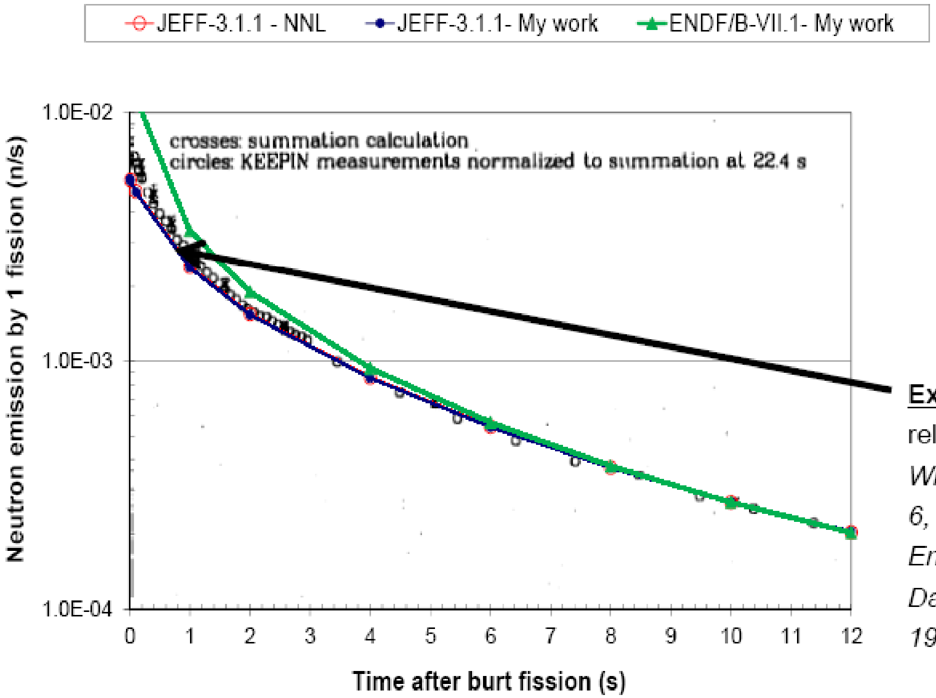
3.1 $n_{emit}(t)$ comparison with EXP.

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.



Experimental values taken from Keepin's relative experiment (*G.R. Keepin, T. R. Wimett, and R. K. Zeigler, J. Nucl. Energy 6, 1(1957)*) Ref: *G. Rudstam, T. R. England, Test of Pre-ENDF/B-VI Decay Data and Fission Yields, LA--II 909-MS, 1990*

1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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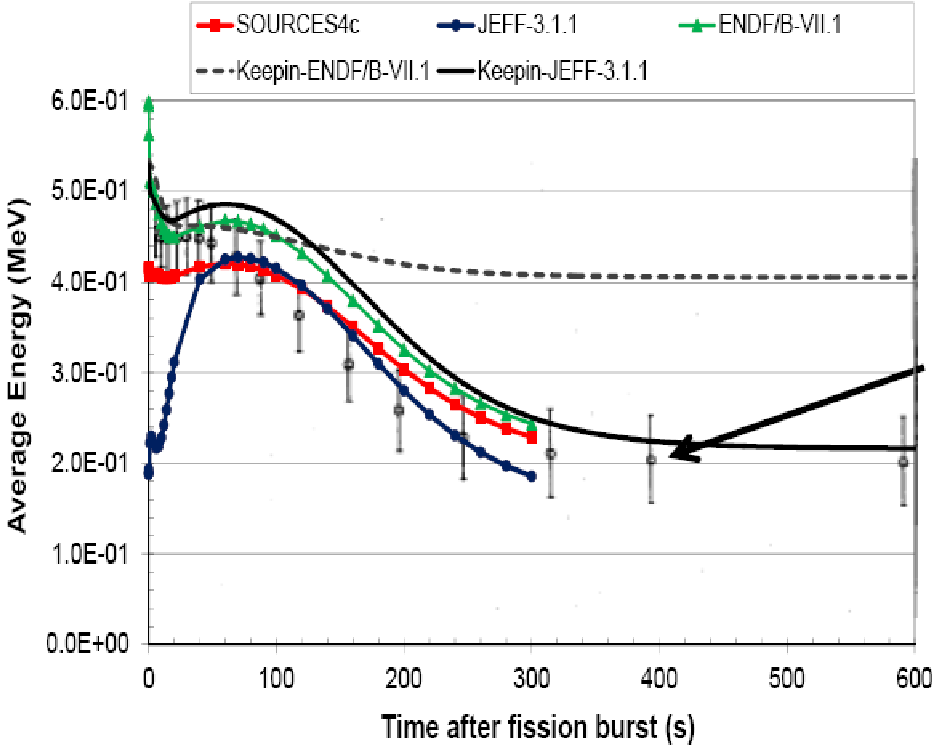
3.3 Delayed Neutron Average Energy

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



__Experimental values__ taken from Ref: *G. Rudstam, T. R. England, Test of Pre-ENDF/B-VI Decay Data and Fission Yields, LA-II 909-MS, 1990,* referenced to Keepin's relative experiment.(*G.R. Keepin, T. R. Wimett, and R. K. Zeigler, J. Nucl. Energy 6, 1(1957)*)

1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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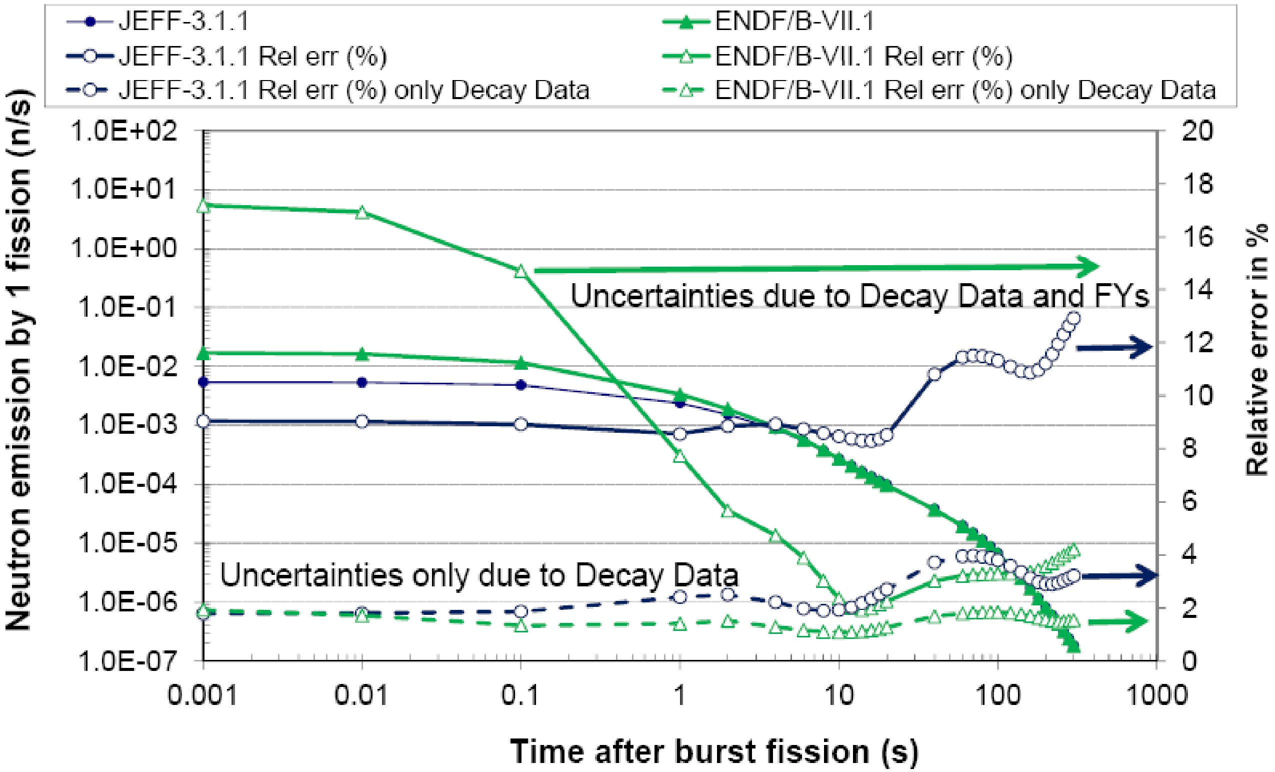
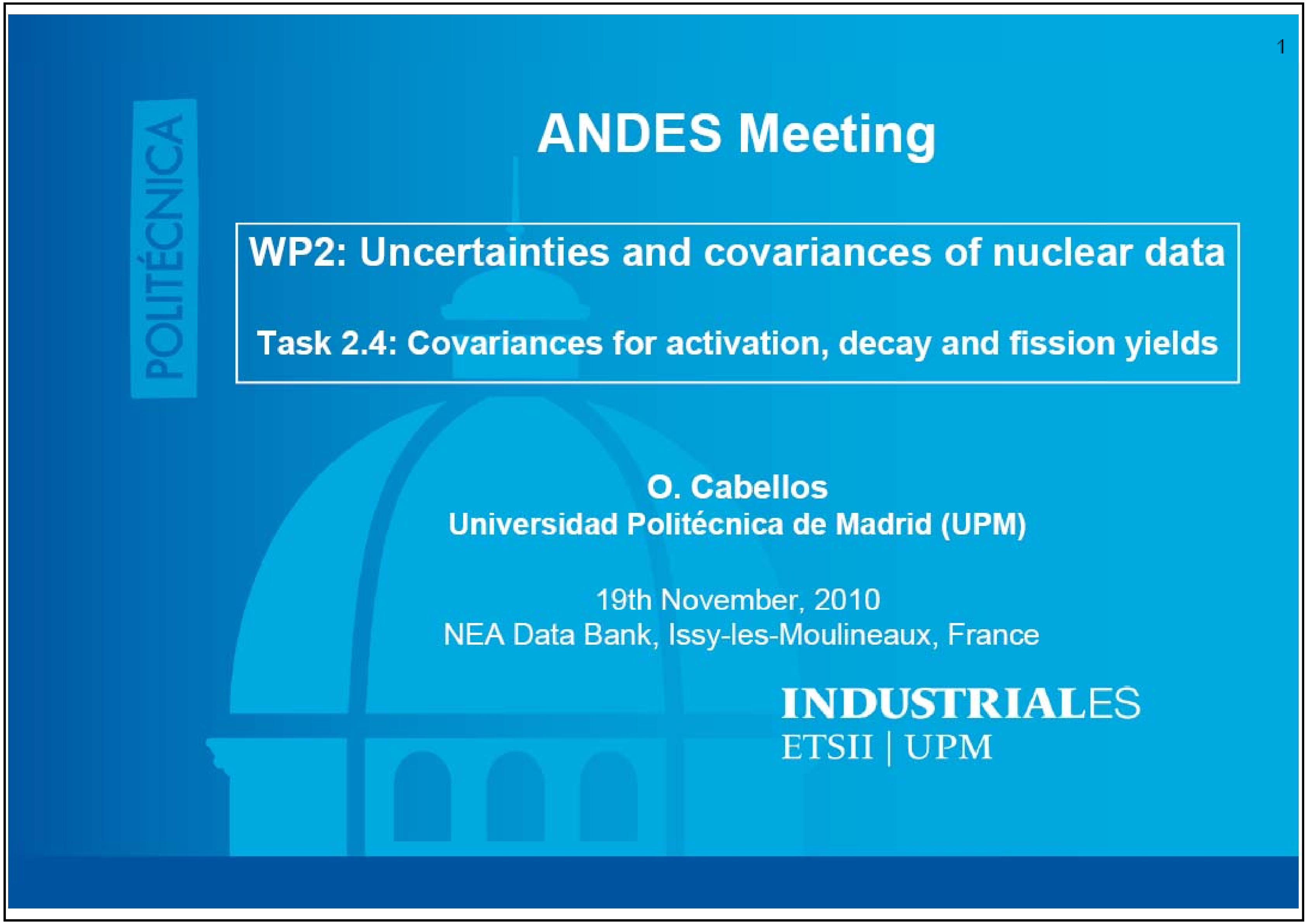
Importance of Decay Data Uncert.

Figure 10. Neutron Emission relative error calculated due to uncertainties in Decay Data and Independent Fission Yields.



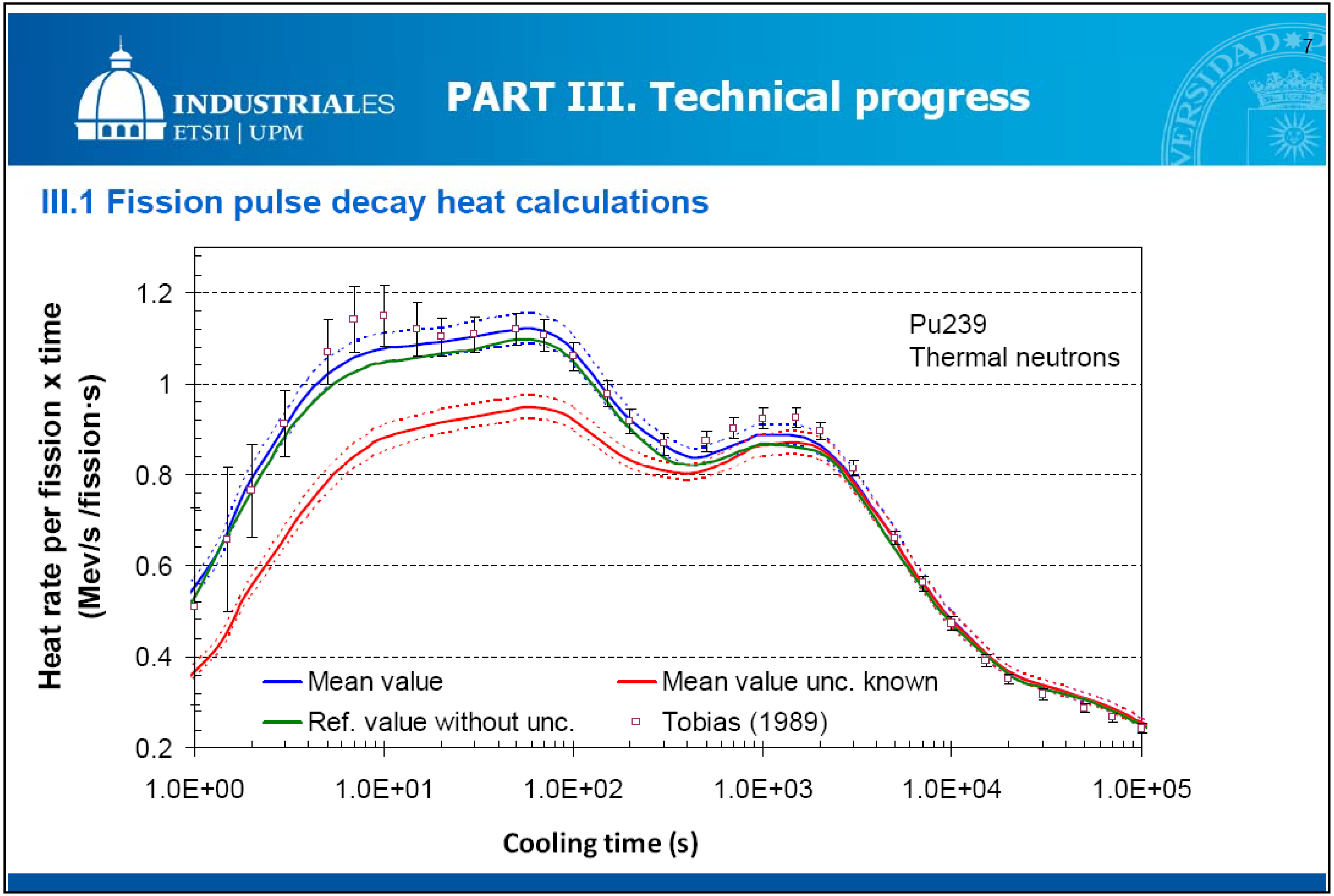
1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)



1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)



1. Processing of nuclear data: JEFF/EFF activities

1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

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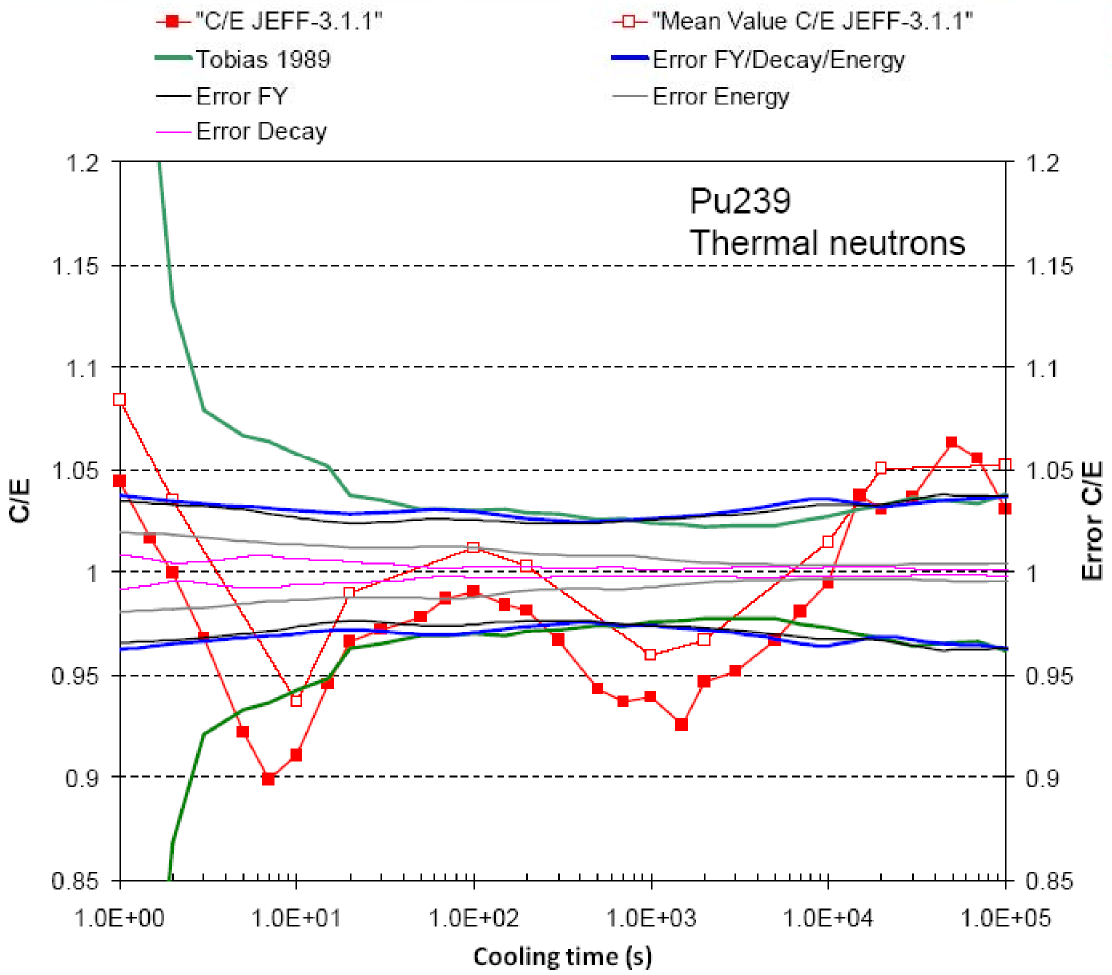
III.1 Fission pulse DH

- For rapid reactor transients, the prediction of DH is important in the range of seconds to minutes
- Identical C/E results reported in JEFF report 20 with FISPIN code
- Tobias (1989) reviewed the status of DH exp. using 45 sets of exp. measurements
- Differences between: "C/E" and "Mean Value C/E"
- It is shown the experimentally derived uncertainties ±1 STD (green line)
- Uncertainties in calculated values are shown: Decay/Energy/FY and Total



Outline

1. Processing of nuclear data: JEFF/EFF activities
   - 1.1 Activities in JEFF: JEFF-3.1,3.11 and 3.1.2 (JEFF-May-2012)
   - 1.2 Activities in EFF : Photonuclear, DPA and STLs (EFF-Nov-2012)
     - 1.2.1 Processed DPA in multigrous, New IAEA/CRP on dpa
   - 1.3 Activities in JEFF/FY: FPDN (JEFF/FY-May-2012) and FPDH (ANDES-Nov-2010)

2. Activation and source term calculation
   - 2.1 Description of ACAB code (NEA-1839, DAE-2010 and EFF-Nov-2009)
   - 2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14-JNM-paper), ADS (Annals-EFIT)
   - 2.3 Applications: Burnup Credit (ICNC-2011, ANS-2011, Annals-paper)
   - 2.4 Other work: Fission Chambers (EFF-May-2012 and NIMA-paper)

3. Uncertainty propagation
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   - 3.2 Uncertainties in depletion calculation (ANS-2011)
   - 3.3 Examples in: IFE, MFE, IFMIF, ADS (ND-2010)
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   - 3.5 Examples in criticality calculations: UAM contributions (UAM5-2011, NCSC2-2011 and UAM6-2012)
   - 3.6 Examples in ESFR: Uncertainty in reactivity coefficients (ND-2013)

4. Summary

2. Activation and source term calculation

2.1 Description of ACAB code (NEA-1839, DAE-2010 and EFF-Nov-2009)

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NEA-1839 ACAB-2008.

ACAB-2008, ACtivation ABacus Code

NAME OR DESIGNATION OF PROGRAM, COMPUTER, DESCRIPTION OF PROGRAM OR FUNCTION, METHODS, RESTRICTIONS, TYPICAL RUNNING TIME, FEATURES, RELATED OR AUXILIARY PROGRAMS, STATUS, REFERENCES, HARDWARE REQUIREMENTS, LANGUAGE, SOFTWARE REQUIREMENTS, OTHER RESTRICTIONS, NAME AND ESTABLISHMENT OF AUTHORS, MATERIAL, CATEGORIES

1. NAME OR DESIGNATION OF PROGRAM: ACAB-2008. [top]

2. COMPUTERS [top]

To submit a request, click below on the link of the version you wish to order. Only liaison officers are authorised to submit online requests. Rules for requesters are available here.

Program name	Package id	Status	Status date
ACAB-2008	NEA-1839/02	Tested	18-MAY-2011

Machines used:

Package ID	Orig. computer	Test computer
NEA-1839/02	Linux-based PC,PC Windows	Linux-based PC

3. DESCRIPTION OF PROGRAM OR FUNCTION [top]

The ACAB code is a computer program designed to perform activation and transmutation calculations for nuclear applications. ACAB has been used to simulate realistic operational scenarios of very different nuclear systems: inertial fusion, magnetic fusion, accelerator driven systems, fission reactors,...

ACAB is able to:
- perform space-dependent inventory calculations allowing for multidimensional neutron flux distributions
- treat decay transitions that proceed from the ground, first, and second isomeric states; all the neutron reactions that may occur are treated in the code

http://www.oecd-nea.org/tools/abstract/detail/nea-1839/

The 2nd DAE-BRNS Workshop on "Covariance Error Matrix and its Applications in Reactor Fuel Cycle and Technology"

POLITÉCNICA

Lesson 2. Exercises with ACAB code. Examples

O. Cabellos
Universidad Politécnica de Madrid (UPM)

INDUSTRIALES
ETSII | UPM

29 November - 3 December, 2010

Vel –Tech Campus, Chennai, India

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1. Introduction

We need "Activation Codes" to predict the **isotopic inventory** under neutron irradiation with energy below 20 MeV and arbitrary operational schedules.

Activation Codes:

USA: ORIGEN , ALARA, DKR, ...
Europe: FISPACT (UK), ACAB (Spain)
Japan: DSCHAIN, ...

Objectives:

- Evaluation of different **Waste Management** options
- Compute response functions for **Safety Analysis**

ACAB code was developed in 80's designed to perform activation and transmutation calculations for fusion applications:

- Validation for Fission/Fusion applications has been performed
- Currently, it has been validated for transmutant systems applications

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2. ACAB Capabilities

- ACAB code is designed to perform activation and transmutation calculations.
- The code solves the general nuclear transmutation chains for multidimensional neutron flux distributions
- ACAB has the ability to simulate realistic operational scenarios of very different systems(e.g., pulsed scheduled for Inertial Fusion)
- Scenarios in which materials are intermittently irradiated, and materials feed instantaneously and/or continuously into the system
- ACAB considers:
  - **Decay transitions** : from ground, first and second isomeric states
  - **Neutron reactions**: All the neutron reactions
  - **Sequential charge particle reactions** as additional mechanisms for the production of activity
  - **Photon** activation, **proton/deuteron** activation.

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7. Computational Benchmark

Initial composition : 1.0E+25 Cr-50 atoms   Irradiation : 1 full power year

Nuclido	FISPACT	REAC	ACT4	RACC	ACAB	DKR	FDKR	IRRADIA	SAM	FRINDA	ANITA
H-1	7.472E+26	0.483	-	-	0.999	-	-	1.000	-	-	1.000
H-2	1.5168E+25	0.993	-	-	0.999	-	-	7.242E+4	-	-	0.999
H-3	8.6940E+20	0.723	-	-	0.998	-	-	0.143	-	-	1.050
He-3	1.6470E+19	0.656	-	-	0.998	-	-	9.116E-2	-	-	0.939
He-4	1.4710E+22	0.779	-	-	0.999	-	-	-	-	-	0.889
Ti-48	5.5482E+23	0.881	0.897	0.612	0.998	1.000	0.988	2.176	-	-	0.965
Ti-49	1.1388E+26	0.999	1.005	0.957	0.999	1.000	0.994	0.999	-	-	0.998
V-49	2.6309E+26	0.999	0.995	0.960	1.000	1.000	0.999	0.998	-	1.003	1.000
V-50	3.8125E+26	1.000	1.011	1.000	1.000	1.000	0.996	1.010	-	0.585	0.999
V-51	1.4167E+26	0.999	0.980	1.000	0.999	1.000	0.990	0.983	-	-	0.999
Cr-50	9.9083E+28	1.000	1.000	1.000	1.000	1.000	1.000	1.008	-	-	1.000
Cr-51	1.6967E+25	1.000	1.001	1.000	1.000	1.000	0.993	1.008	1.060	1.009	0.999
Cr-52	4.3766E+22	0.779	1.115	1.000	1.000	1.000	0.989	3.798E-2	-	-	0.889
Cr-53	1.1985E+19	0.712	-	1.000	0.999	1.000	0.916	-	-	-	0.855
Cr-54	6.2966E+15	0.614	-	1.000	0.998	1.000	-	-	-	-	0.801

ε max FISPACT/other		REAC	ACT4	RACC	ACAB	DKR	FDKR	IRRADIA	SAM	FRINDA	ANITA
	Light Nuclides	52%		NO	0.2%	NO					11%
	Nuclides in Ground state	39%		39%	0.2%	0%					20%

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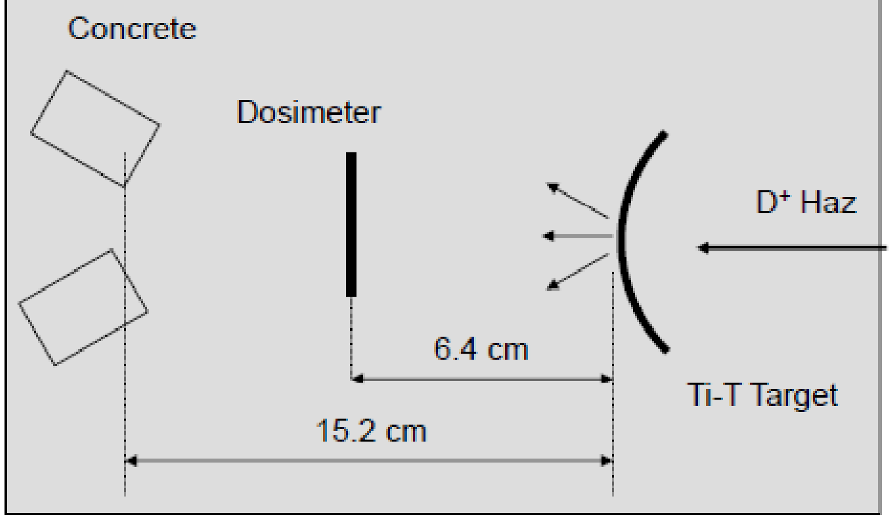
7. Integral Experiments for validation of modelling of the NIF chamber : TART/ACAB

Concrete Composition, no-borated, of NIF. Borated is similar with 0.01% of boron.

Element	Atomic (%)	Element	Atomic (%)
H	13.465	B	0.001
C	0.599	O	60.576
Na	0.519	Mg	0.286
Al	1.687	Si	11.056
S	0.213	K	0.599
Ca	6.987	Sc	0.000046
Ti	0.037	Cr	0.002
Mn	0.00072	Fe	0.336
Ni	0.00059	Cu	0.00028

Irradiation Facility

(Rotating Target Neutron Source, U.C. Berkeley)



Concrete Dimensions

Sample	Diameter (cm)	Height (cm)	Volume (cm^3)
Borated	10.16	10.21	3311.29
NoBorated	10.19	10.16	3310.48

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

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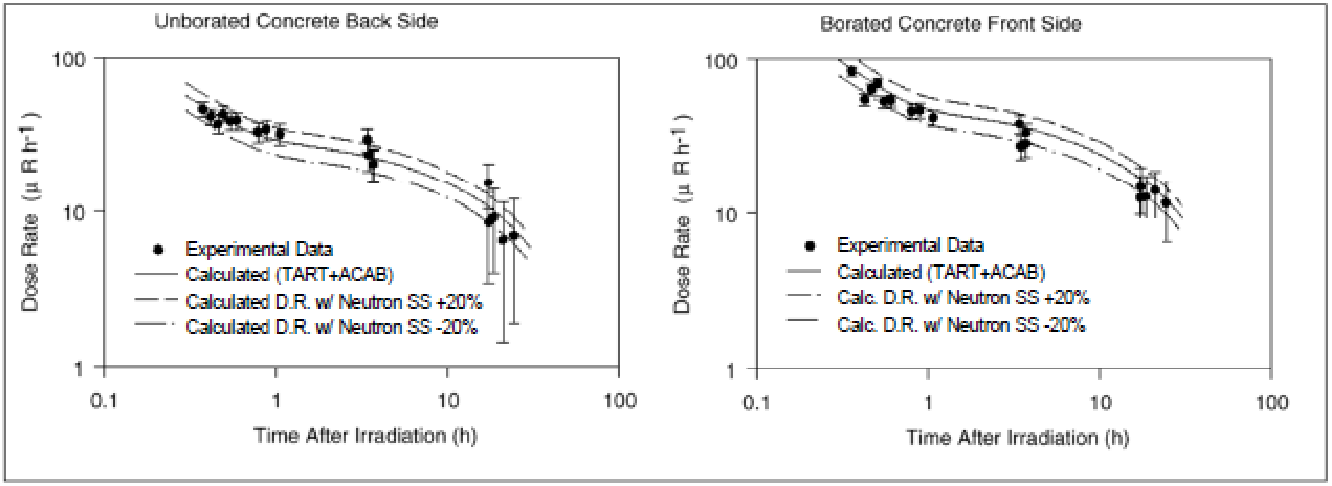
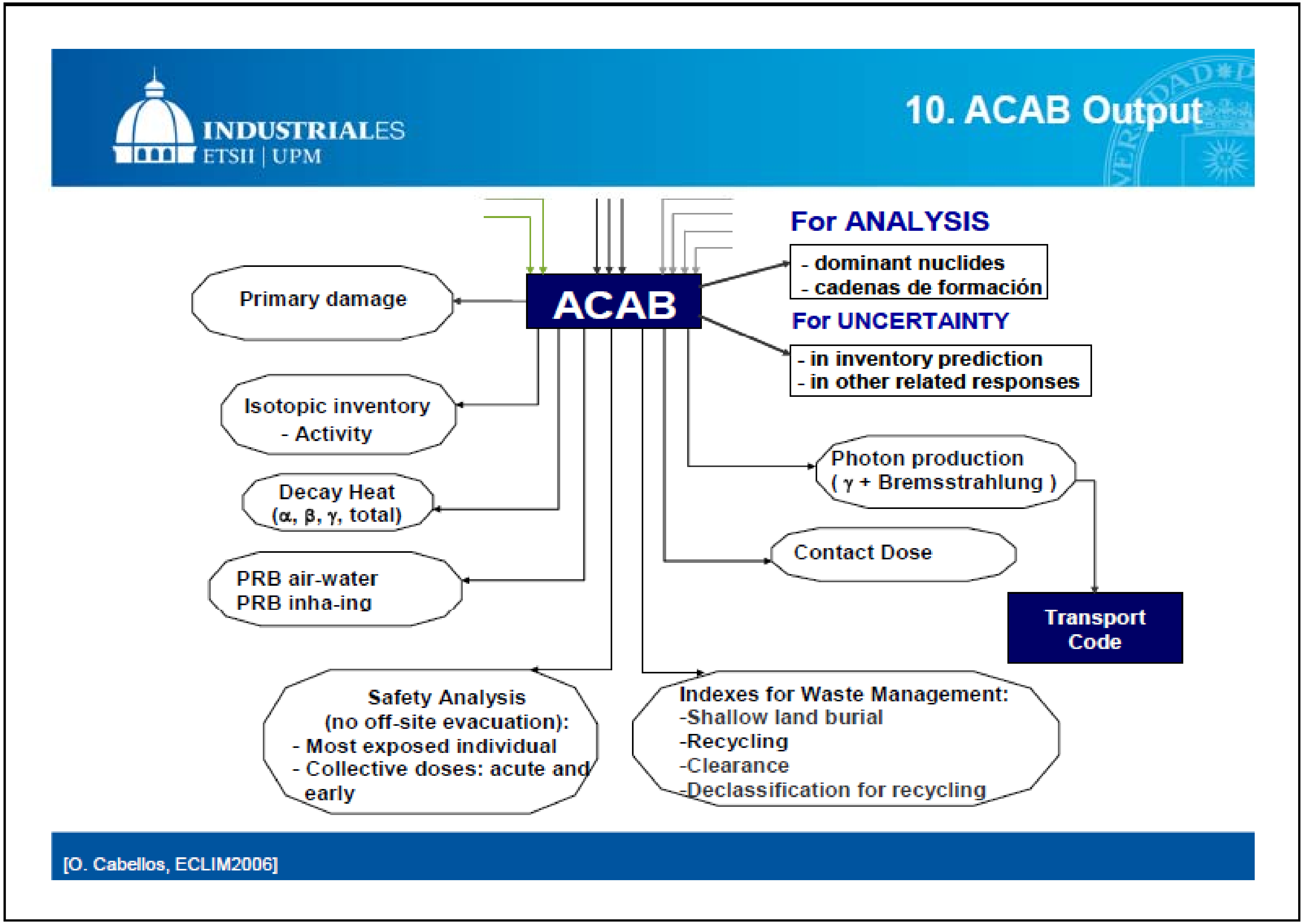
7. Integral Experiments for validation of modelling of the NIF chamber : TART/ACAB





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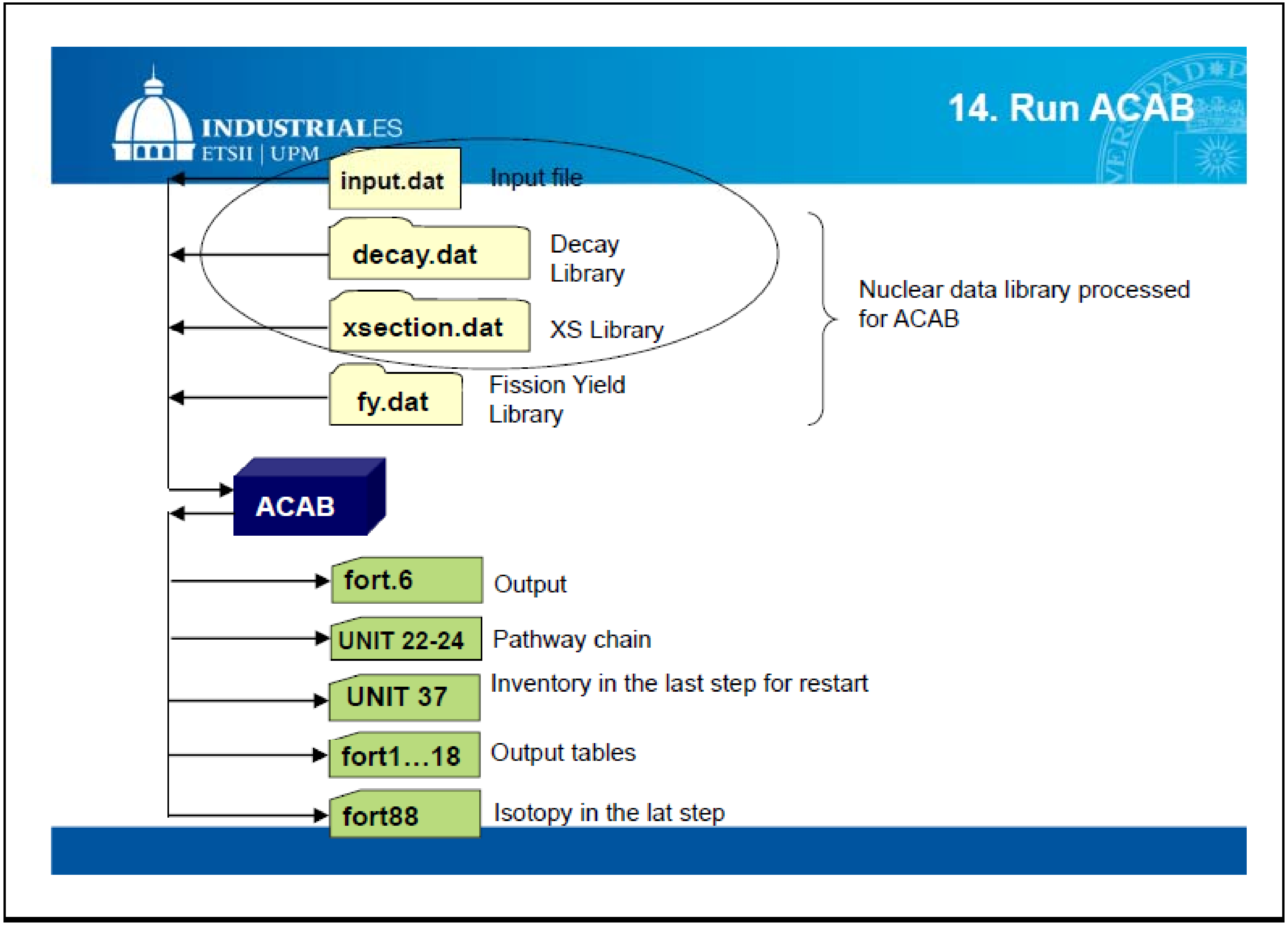
10. ACAB Output
For ANALYSIS
- dominant nuclides
- cadenas de formación
For UNCERTAINTY
- in inventory prediction
- in other related responses
ACAB
Primary damage
Isotopic inventory
- Activity
Decay Heat
(α, β, γ, total)
PRB air-water
PRB inha-ing
Photon production
(γ + Bremsstrahlung)
Contact Dose
Transport
Code
Safety Analysis
(no off-site evacuation):
- Most exposed individual
- Collective doses: acute and early
Indexes for Waste Management:
-Shallow land burial
-Recycling
-Clearance
-Declassification for recycling
[O. Cabellos, ECLIM2006]



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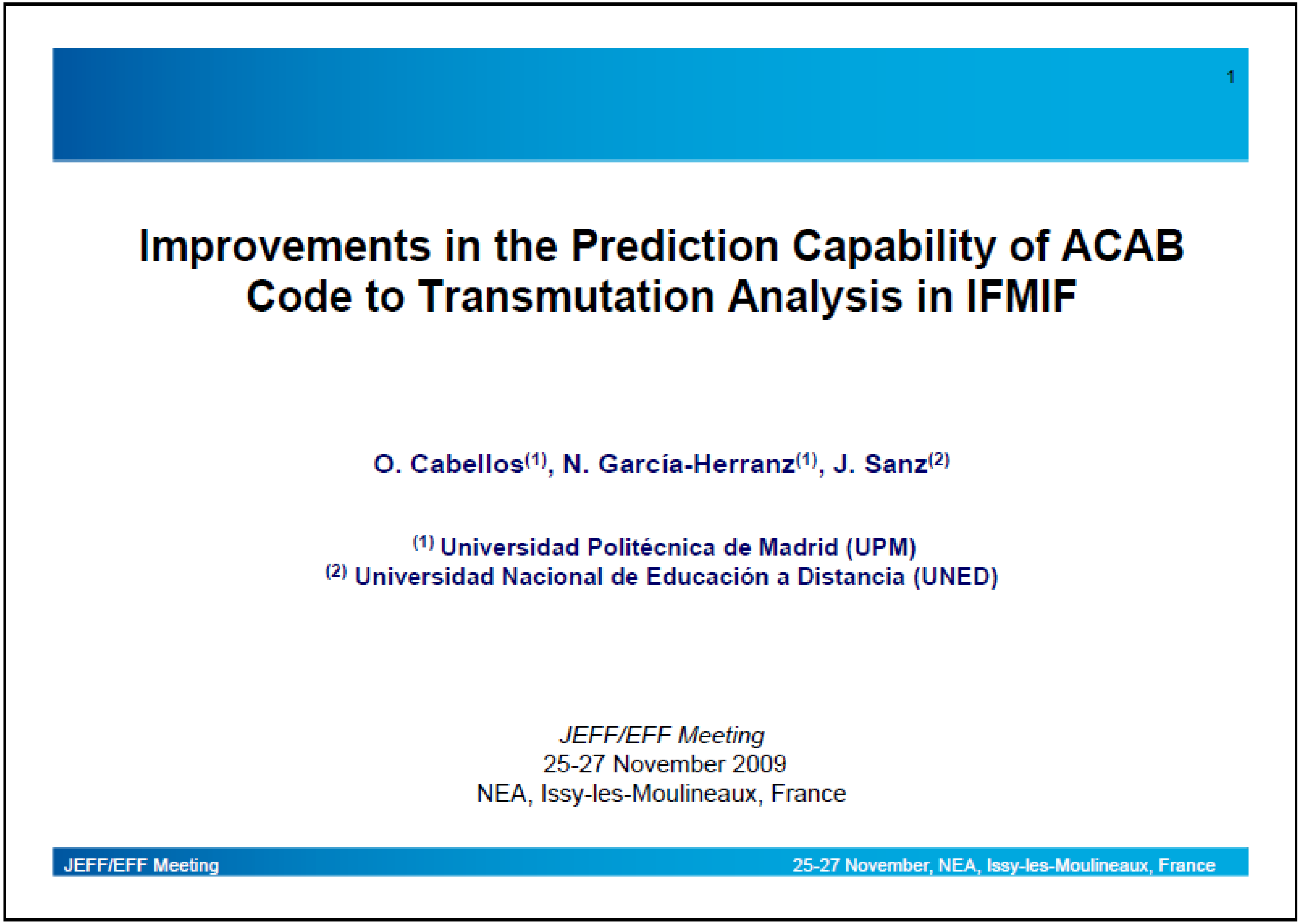
14. Run ACAB
input.dat
Input file
decay.dat
Decay Library
xsection.dat
XS Library
fy.dat
Fission Yield Library
Nuclear data library processed for ACAB
ACAB
fort.6
Output
UNIT 22-24
Pathway chain
UNIT 37
Inventory in the last step for restart
fort1…18
Output tables
fort88
Isotopy in the lat step

2. Activation and source term calculation

2.1 Description of ACAB code (NEA-1839, DAE-2010 and EFF-Nov-2009)



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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

PART II. Prediction of atomic displacements (dpas)

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$$\frac{dpa}{s} = \sum_i \rho^i \cdot \phi \cdot \frac{\sigma^i_{Damage}}{2E^i_d}$$

- ρ^i = f(time) is the number density of nuclide i
- ϕ is the total neutron flux
- σ^i_D (eV-b) is the 1group damage energy production XS of nuclide i
- E^i_d is the energy required to displace the atom i from its lattice
- the sum is extended over all isotopes

- We have processed a 211-multigroup damage library from **ENDF/B-VII.0** with NJOY99.220

  (NEA Data Bank /processing data/, December 2007)

		IFMIF					DEMO					HYLIFEII				
Z	Element	DPA	H	ε%	He	ε%	DPA	H	ε%	He	ε%	DPA	H	ε%	He	ε%
5	B	18	806	7	3474	7	39	739	10	54250	6	24	38	12	64376	5
6	C	0	423	16	3431	39	0	3	7	3964	56	0	0	6	108	48
7	N	25	2683	12	2468	12	30	3831	19	1829	27	4	355	7	137	6
8	O	35	359	10	1397	8	41	412	5	1200	7	5	8	4	70	7
13	Al	47	1084	9	703	10	48	1425	9	962	14	5	45	5	33	16
14	Si	55	2309	4	1202	4	55	2487	2	1472	3	5	85	2	58	3
15	P	54	3936	17	880	14	52	5596	26	1087	10	5	187	19	45	4
16	S	50	4281	8	2662	13	54	4056	13	2873	22	5	206	6	185	13
22	Ti	44	986	8	415	32	52	795	6	274	5	6	25	3	7	6
23	V	0	659	10	81	7	0	738	2	105	2	0	22	2	2	2
24	Cr	40	1143	6	300	12	38	1167	4	235	13	3	35	3	8	23
25	Mn	33	844	17	197	31	39	713	20	163	5	4	18	15	4	5
26	Fe	38	1445	7	293	5	38	1452	2	318	2	3	47	2	10	3
27	Co	37	1249	17	259	27	43	1827	16	241	8	4	43	15	7	4
28	Ni	50	5787	6	1808	29	51	7118	5	1290	11	5	830	12	500	22
29	Cu	51	2030	17	317	5	51	2170	26	331	6	4	97	21	10	7
39	Y	51	789	16	52	8	60	898	26	37	5	5	27	27	1	5
41	Nb	19	738	15	120	17	20	520	8	113	4	2	13	7	3	4
42	Mo	19	1120	12	104	9	23	1241	25	94	7	2	28	19	2	6
73	Ta	10	193	24	19	26	12	31	7	4	6	1	1	13	0	12
74	W	12	224	10	26	12	11	42	10	343	30	1	2	9	965	29

Table. Damage (in dpas), gas production rates for H and He (appm) and relative error (ε, in %) of typical intended and impurities elements in reduced activation steels after 1 fpy in HFTM/IFMIF, DEMO and HYLIFEII.

PART II. DPA and ratios H/dpa and He/dpa for iron (Fe)

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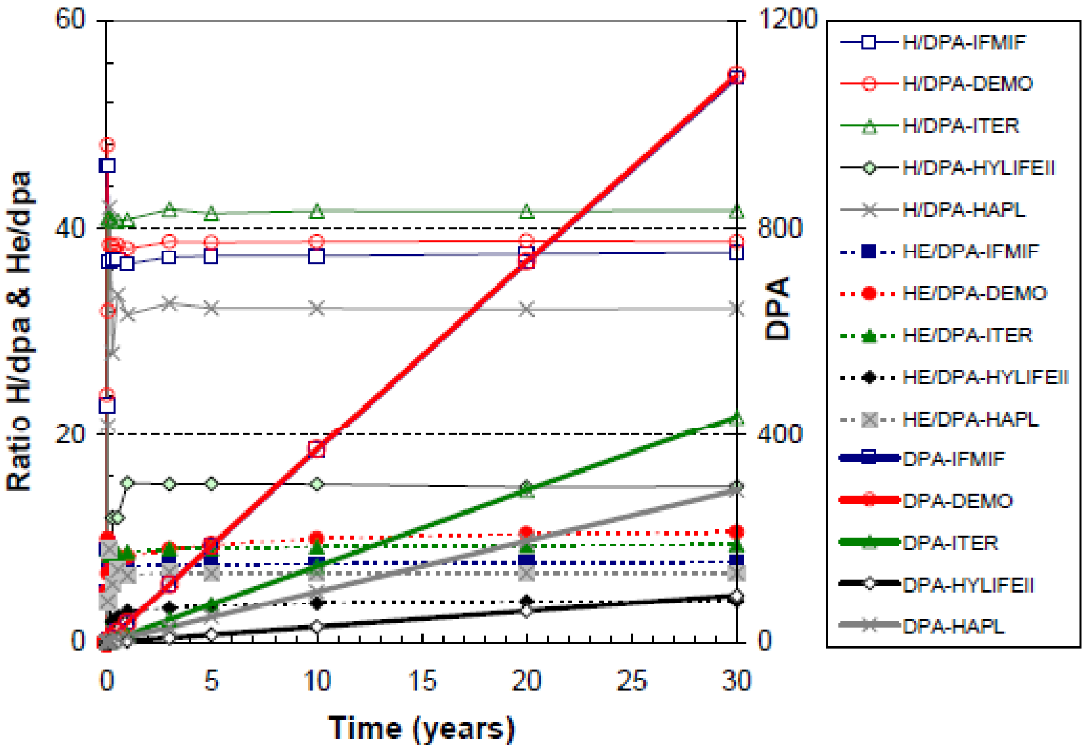
- For Fe, in HFTM, the dpa rate is 1.19x10^{-6} dpa/s, and after 1 fpy of irradiation this value decrease in 0.4%



2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14 and JNM-paper), ADS (Annals-EFIT)

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Fusion Engineering and Design

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Effect of activation cross-section uncertainties in selecting steels for the HYLIFE-II chamber to successful waste management

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Available online 26 July 2005

Abstract

We perform the waste management assessment of the different types of steels proposed as structural material for the inertial fusion energy (IFE) HYLIFE-II concept. Both recycling options, hands-on (HoR) and remote (RR), are unacceptable. Regarding shallow land burial (SLB), 304SS has a very good performance, and both Cr–W ferritic steels (FS) and oxide-dispersion-strengthened (ODS) FS are very likely to be acceptable. The only two impurity elements that question the possibility of obtaining reduced activation (RA) steels for SLB are niobium and molybdenum. The effect of activation cross-section uncertainties on SLB assessments is proved to be important. The necessary improvement of some tungsten and niobium cross-sections is justified.

Keywords: IFE; HYLIFE II; Waste management; Low activation steels; Cross-section uncertainties

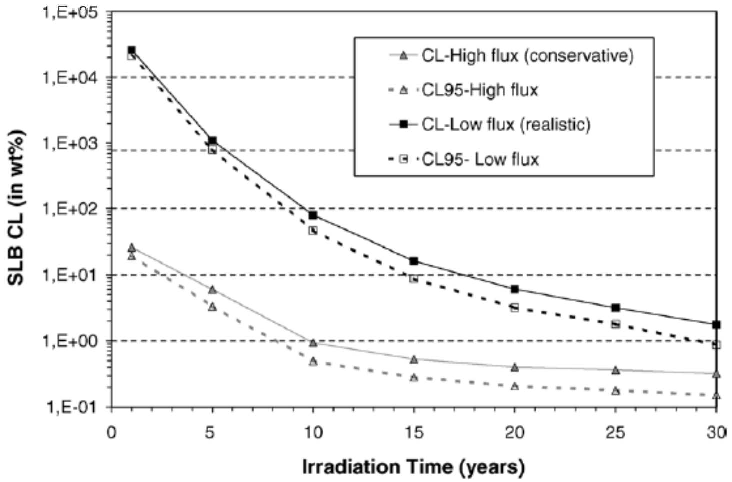

Fig. 1. Tungsten CL for SLB as function of irradiation time for two different neutron flux intensities. Uncertainties (CL95) are also provided

2. Activation and source term calculation

2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14 and JNM-paper), ADS (Annals-EFIT)

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Fusion Engineering and Design 81 (2006) 1561–1565

Fusion Engineering and Design

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Effect of activation cross-section uncertainties on the radiological assessment of the MFE/DEMO first wall

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Available online 27 December 2005

Abstract

A Monte Carlo procedure has been applied in this work in order to address the impact of activation cross-sections (XS) uncertainties on contact dose rate and decay heat calculations for the outboard first wall (FW) of a magnetic fusion energy (MFE) demonstration (DEMO) reactor. The XSs inducing the major uncertainty in the prediction of activation related quantities have been identified. Results have shown that for times corresponding to maintenance activities the uncertainties effect is insignificant since the dominant XSs involved in these calculations are based on accurate experimental data evaluations. However, for times corresponding to waste management/recycling activities, the errors induced by the XSs uncertainties, which in this case are evaluated using systematic models, must be considered. It has been found that two particular isotopes, ^{60}Co and ^{94}Nb, are key contributors to the global DEMO FW activation uncertainty results. In these cases, the benefit from further improvements in the accuracy of the critical reaction XSs is discussed.

Keywords: DEMO; Activation cross-section; Uncertainty analysis

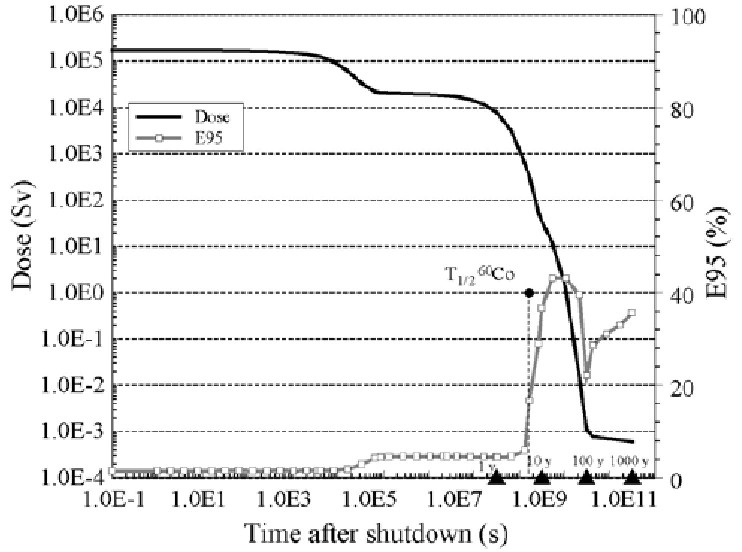

Fig. 1. Contact dose rate and relative error (E_{95}) for the outboard DEMO blanket FW.

2. Activation and source term calculation

2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14 and JNM-paper), ADS (Annals-EFIT)

Journal of Nuclear Materials 417 (2011) 1307–1310

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Impact of activation cross-section uncertainties on the tritium production in the HFTM specimen cells

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ARTICLE INFO

Article history:
Available online 1 January 2011

ABSTRACT

The prediction of the tritium production is required for handling procedures of samples, safety & maintenance and licensing of the International Fusion Materials Irradiation Facility (IFMIF). A comparison of the evaluated tritium production cross-sections with available experimental data from the EXFOR data base has shown insufficient validation. And significant discrepancies in evaluated cross-section libraries, including lack of tritium production reactions for some important elements, were found.

Here, we have addressed an uncertainty analysis to draw conclusions on the reliability of the tritium prediction under the potential impact of activation cross-section uncertainties. We conclude that there is not sufficient experimental validation of the evaluated tritium production cross-sections, especially for iron and sodium. Therefore a dedicated experimental validation program for those elements should be desirable.

PART III. Problem description

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- The tritium production in the HFTM specimen cells

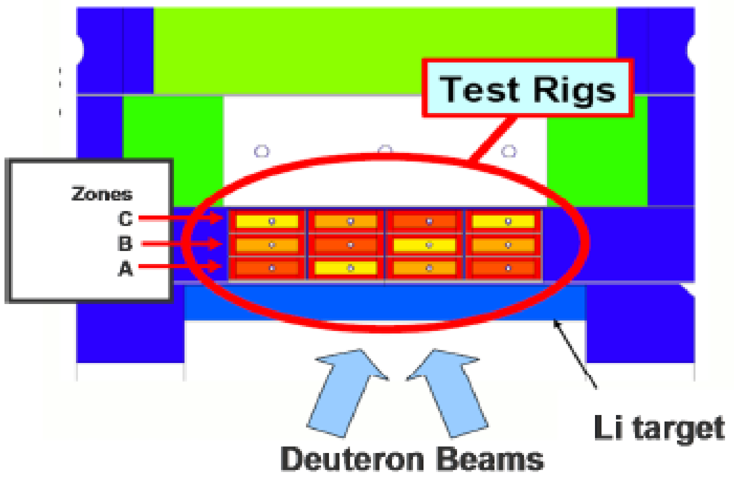

Table 1. Initial composition (in % atom fraction) for the three test rigs

Element	Rig-1	Rig-2	Rig-3
Cr	7.1	9.3	7.9
C	0.40	0.5	0.4
Mn	0.30	0.39	0.33
V	0.26	0.21	0.18
W	0.22	0.29	0.25
Ta	0.016	0.021	0.018
Fe	65.50	86.0	73.4
Na	18.0	2.3	12.0
K	8.30	1.0	5.5

- The McDeLicious code to compute the neutron flux
- The ACAB-2008 code to perform activation calculations

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PART III. UA on the T production in the HFTM specimen cells

- **Uncertainty calculation**
  - nominal value (Ci/fpy) calculated with the best-estimate XS data
  - mean value (Ci/fpy) and standard deviation (Ci/fpy) calculated with the uncertainty library using the Monte Carlo method with ACAB code

Table 3 Tritium production calculated with EAF2007

0.6 0.7±0.3	0.8 1.0±0.5	0.7 0.9±0.3	0.6 0.7±0.3
0.9 1.1±0.6	1 1.2±0.5	0.9 1.1±0.4	0.9 1.1±0.6
1.1 1.4±0.5	1.2 1.4±0.5	1.3 1.6±0.9	1.1 1.4±0.5

Nominal value (Ci/fpy)
Mean ± s.d. (Ci/fpy)

- **Total tritium prediction:**
  - **IEAF2001:** 23.4 Ci/fpy
  - **EAF-2007:** 11.2 Ci/fpy (best-estimate)
  - **EAF2007/UN:** 13,7± 6 (Uncertainties)
  - Relative errors up to 51% in tritium prediction can be found in rig 2
  - Similar relative errors for the same rigs positioned in different locations
  - Histogram of the Monte Carlo sampling fit to a long tail lognormal distribution

2. Activation and source term calculation

2.2 Applications: IFE(SOFT2004), MFE(ISTN-2005), IFMIF(ICFRM14 and JNM-paper), ADS (Annals-EFIT)

Annals of Nuclear Energy 37 (2010) 1570–1579

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Nuclear data requirements for the ADS conceptual design EFIT: Uncertainty and sensitivity study

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ABSTRACT

In this paper, we assess the impact of activation cross-section uncertainties on relevant fuel cycle parameters for a conceptual design of a modular European Facility for Industrial Transmutation (EFIT) with a "double strata" fuel cycle. Next, the nuclear data requirements are evaluated so that the parameters can meet the assigned design target accuracies. Different discharge burn-up levels are considered: a low burn-up, corresponding to the equilibrium cycle, and a high burn-up level, simulating the effects on the fuel of the multi-recycling scenario.

In order to perform this study, we propose a methodology in two steps. Firstly, we compute the uncertainties on the system parameters by using a Monte Carlo simulation, as it is considered the most reliable approach to address this problem. Secondly, the analysis of the results is performed by a sensitivity technique, in order to identify the relevant reaction channels and prioritize the data improvement needs. Cross-section uncertainties are taken from the EAF-2007/UN library since it includes data for all the actinides potentially present in the irradiated fuel.

Relevant uncertainties in some of the fuel cycle parameters have been obtained, and we conclude with recommendations for future nuclear data measurement programs, beyond the specific results obtained with the present nuclear data files and the limited available covariance information. A comparison with the uncertainty and accuracy analysis recently published by the WPEC-Subgroup26 of the OECD using BOLNA covariance matrices is performed. Despite the differences in the transmuter reactor used for the analysis, some conclusions obtained by Subgroup26 are qualitatively corroborated, and improvements for additional cross sections are suggested.

Table 3
Nominal values and uncertainties in the total decay heat along cooling time.

Time (years)	150 GWd/tHM		500 GWd/tHM	
	Nominal value (W)	Uncertainty (%)	Nominal value (W)	Uncertainty (%)
Shutdown	1.58E+07	3.63	9.27E+06	1.77
1	7.79E+05	4.68	5.42E+05	7.49
10	3.51E+05	4.02	2.93E+05	9.83
100	8.11E+04	2.37	4.73E+04	6.51
1000	1.10E+04	2.45	6.37E+03	5.76
10,000	2.62E+03	1.32	1.68E+03	4.38
100,000	2.55E+02	2.37	1.45E+02	6.24

Table 6
Most relevant nuclides and uncertainties in its concentration. (T: transmutation; DH: decay heat, N: neutron emission, R: radiotoxicity).

Nuclide	Uncertainty in concentration (%) Burn-up (GWd/tHM)		Relevant in			
	150	500				
U-234	4.6	16.1	T	DH		
U-235	13.1	18.4	T			
U-236	1.8	7.6	T			
Np-237	6.3	23.7	T			
Pu-238	4.3	10.8	T	DH		R
Pu-239	4.6	12.9	T	DH		R
Pu-240	2.0	7.0	T	DH		R
Pu-241	8.2	14.7	T			
Pu-242	2.1	7.9	T	DH		R
Am-241	7.2	20.7	T	DH		R
Am-242m	12.8	28.6	T			
Am-243	6.6	15.6	T	DH		R
Cm-242	10.7	7.7	T	DH		
Cm-243	23.3	32.6	T			
Cm-244	6.0	13.3	T	DH	N	R
Cm-245	13.3	18.8	T			
Cm-246	7.5	21.7	T		N	
Cm-247	15.4	27.2	T			
Cm-248	6.4	19.8			N	
Cf-250	31.9	28.9			N	
Cf-252	52.4	46.1			N	

Table 8

Uncertainties (in%) in response functions due to uncertainties in each cross section contributing with an uncertainty larger than 0.5%. Sensitivity calculations correspond to the discharge, for a burn-up of 500 GWd/tHM. (DH-100y: decay heat after 100 years cooling time, N-2y: neutron emission after 2 years cooling time, INH-10,000y: CEDE by inhalation after 10,000 years cooling time).

		Response function		
		DH–100y	N-2y	INH-10,000y
Uncertainty due to				
Np^{237}	Fission	0.53		
	(n,γ)	0.55		0.28
Pu^{238}	Fission	1.98		0.51
	(n,γ)	1.90		0.75
Pu^{239}	Fission	0.39		0.93
	(n,γ)	0.53		0.94
Pu^{240}	Fission	0.93		1.50
	(n,γ)	1.28		1.72
Pu^{241}	Fission	1.78	0.28	0.50
	(n,γ)	0.90	0.34	0.62
Pu^{242}	Fission	0.34	0.33	0.62
	(n,γ)	0.89	0.91	1.44
Am^{241}	Fission	0.71		
	(n,γ)	1.43		0.44
	$(n,\gamma-M)$	0.63		
Am^{242m}	Fission	0.70		0.27
	(n,γ)	0.37		0.32
Am^{243}	Fission	0.40	0.40	0.64
	(n,γ)			0.47
	$(n,\gamma-M)$	0.92	0.90	1.78
Cm^{242}	Fission	0.41		
	(n,γ)	0.64		
Cm^{243}	Fission			
	(n,γ)			
Cm^{244}	Fission	0.74	0.80	0.91
	(n,γ)	1.42	1.61	1.90
Cm^{245}	Fission		0.40	0.84
	(n,γ)	0.32	1.00	0.93

Table 9

One-group uncertainties in the critical cross sections processed from EAF-2007/UN (Δ_{EAF}), uncertainties required for satisfying the target accuracies (Δ_{target}) and required uncertainty reduction ($\Delta_{EAF}/\Delta_{target}$). Calculations correspond to a burn-up of 500 GWd/tHM.

Reaction		Δ_{EAF}	Δ_{TARGET}	$\Delta_{EAF/DTARGET}$
U^{234}	(n,γ)	38.9	7.1	5
	$(n,\gamma-M)$	38.9	7.1	5
U^{235}	Fission	12.9	4.2	3
Np^{237}	(n,γ)	14.3	2.8	5
Pu^{238}	Fission	12.3	6.4	2
	(n,γ)	14.5	5.2	3
Pu^{239}	Fission	9.6	3.4	3
Pu^{240}	(n,γ)	9.3	4.8	2
Pu^{241}	Fission	15.6	4.2	4
Pu^{242}	(n,γ)	12.6	5.3	2
Am^{241}	(n,γ)	15.8	2.8	6
	$(n,\gamma-M)$	15.9	2.9	5
Am^{242m}	Fission	24.0	2.4	10
	(n,γ)	32.8	6.2	5
Am^{243}	$(n,\gamma-M)$	15.3	4.1	4
Cm^{242}	(n,γ)	30.0	3.4	9
Cm^{243}	Fission	16.0	3.2	5
	(n,γ)	32.0	7.4	4
Cm^{244}	(n,γ)	24.6	4.6	5
Cm^{245}	Fission	9.7	4.1	2
	(n,γ)	32.7	5.5	6
Cm^{246}	(n,γ)	28.2	4.3	7
Cm^{247}	Fission	16.5	4.0	4
	(n,γ)	32.1	5.0	6
Cm^{248}	(n,γ)	19.2	2.5	8
Bk^{249}	(n,γ)	31.7	3.2	10
Cf^{249}	(n,γ)	32.4	4.3	7
Cf^{250}	Fission	33.0	6.9	5
	(n,γ)	29.3	2.6	11
Cf^{251}	Fission	31.6	3.7	9
	(n,γ)	29.9	2.4	12

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Impact of Nuclear Data Uncertainties in the Phase-1B Benchmark

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Hollywood, Florida (USA)

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2.1 Phase I-B Burnup Credit Benchmark: "Revisiting the problem"

Table I. Comparison (C/E-1)*100% for different codes for the OECD/NEA Burnup Credit Benchmark Phase-1B (CASE A- 27.35 GWd/TU).

Isotope	WIMSD5	SCALE 6.0		SERPENT1.1.7		Monteburns2.0	MCNP+ACAB	
	LIB1986	NITAWL LIB-44g	CENTRM LIB-238g	All ND taken from JEFF-3.1.1	All ND taken from ENDF/B-VII	ENDF/B-VII + PWRLIB	ENDF/B-VII + EAF2007 + JEFF-3.1.1 Decay&FY	
^{234}U	-2.5	-0.8	0.8	-0.9	-0.9	0.8	0.8	
^{235}U	-3.7	-3.0	-1.1	-3.2	-3.0	-2.7	-2.8	< 3%
^{236}U	0.7	2.0	1.1	1.5	1.7	4.1	4.1	
^{238}U	-0.6	-0.6	-0.6	-0.6	-0.6	1.5	1.5	
^{237}Np	-4.1	3.5	-2.9	4.7	4.0	8.3	7.2	
^{238}Pu	-36.4	-13.8	-20.2	-9.9	-12.6	-10.1	-13.6	
^{239}Pu	-3.5	0.3	3.6	-3.1	-2.9	-0.4	-0.1	< 3%
^{240}Pu	1.4	-1.3	0.4	-0.9	-1.7	0.4	0.4	
^{241}Pu	-4.4	-4.1	-0.3	-2.5	-1.8	-0.9	-0.7	
^{242}Pu	-9.6	-0.5	-3.0	1.4	-0.02	1.0	1.0	
^{241}Am(*)	-3.9	-3.6	0.1	-4.0	-1.5	-1.4	0.3	
^{243}Am(*)	-8.1	14.2	8.2	3.3	12.8	13.9	38.4	

(*) Differences respect to the averaged of the calculated concentrations

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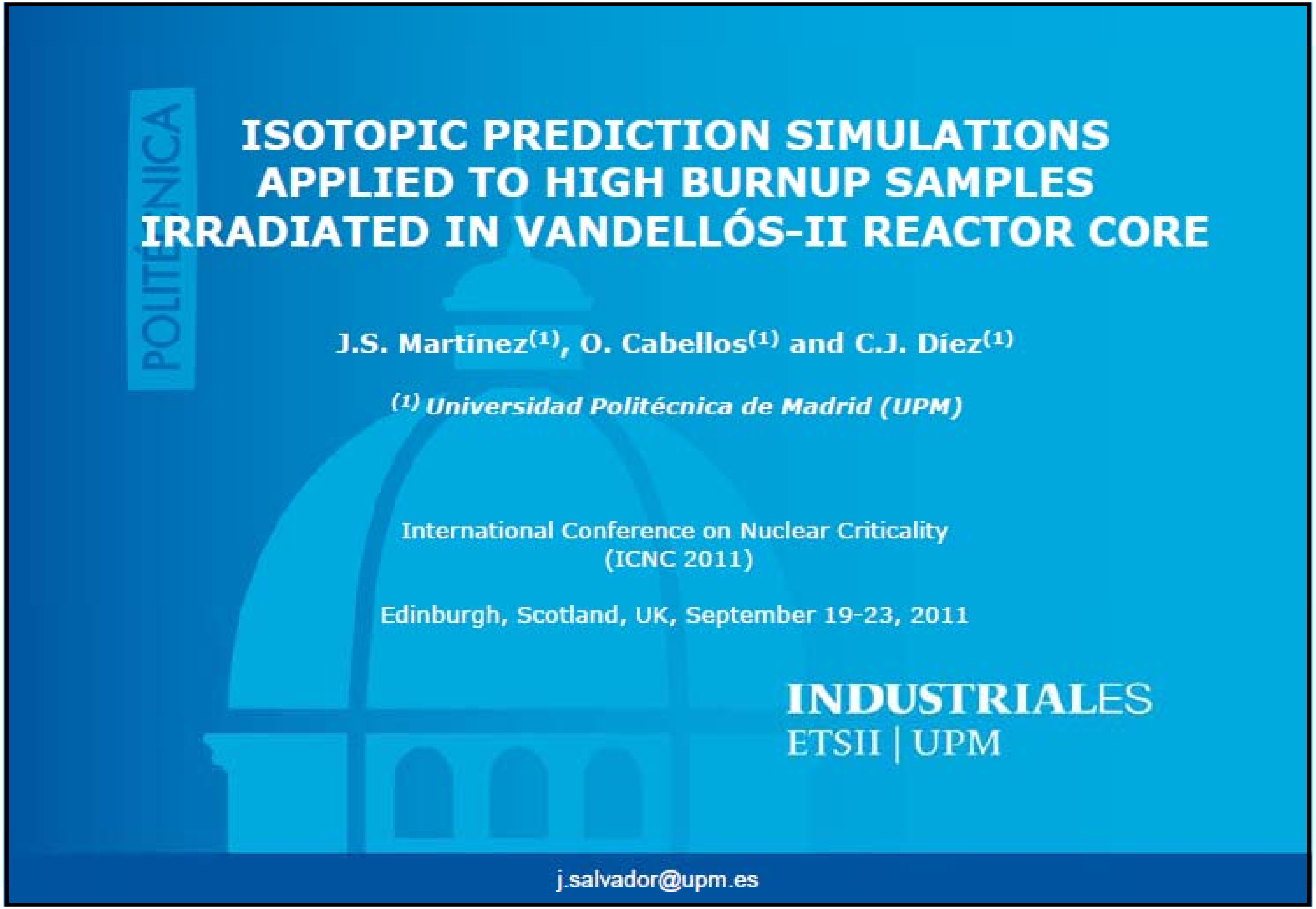
2.1 Phase I-B Burnup Credit Benchmark: "Revisiting the problem: CASE A"

Table II. Comparison (C/E-1)*100% for different codes for the OECD/NEA Burnup Credit Benchmark Phase-1B (**CASE A**- 27.35 GWd/TU).

Isotope	WIMSD5	SCALE 6.0		SERPENT1.1.7		Monteburns2.0	MCNP+ACAB
	LIB1986	NITAWL LIB-44g	CENTRM LIB-238g	All ND taken from JEFF-3.1.1	All ND taken from ENDF/B-VII	ENDF/B-VII + PWRLIB	ENDF/B-VII + EAF2007 + JEFF-3.1.1 Decay&FY
^{95}Mo(*)	2.3	-0.5	-1.0	0.7	0.1	2.1	3.2
^{99}Tc (*)	2.0	0.2	-0.1	-1.5	-1.7	1.4	4.5
^{101}Ru(*)	-0.3	1.3	0.5	2.2	1.3	3.0	4.7
^{103}Rh(*)	-4.9	2.9	3.2	2.5	2.8	4.6	7.4
^{109}Ag(*)	-9.6	-12.9	-11.7	-6.7	-39.1	0.4	10.4
^{133}Cs	-0.5	0.9	0.1	-1.2	0.1	2.6	2.7
^{143}Nd	3.0	0.1	0.0	-0.8	-0.6	2.0	2.5
^{145}Nd	-1.2	-0.4	-1.5	0.7	-0.8	1.6	2.1
^{147}Sm(*)	-4.1	3.2	6.8	5.5	5.3	6.6	3.4
^{149}Sm	-19.4	-33.4	-34.9	-36.5	-35.2	-35.1	-34.6
^{150}Sm	-3.3	-6.7	-1.4	-4.1	-5.5	0.2	-4.3
^{151}Sm(*)	45.7	-0.4	-18.8	-18.3	-19.9	-11.4	-19.4
^{152}Sm	12.1	12.1	-1.2	-0.7	-2.6	7.8	1.3
^{153}Eu	-13.6	-2.3	1.2	2.0	1.8	10.2	4.1
^{155}Gd(*)	-	-52.7	-31.0	-29.2	-30.6	-28.5	-29.9

(*) Differences respect to the averaged of the calculated concentrations



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ISOTOPIC PREDICTION SIMULATIONS APPLIED TO HIGH BURNUP SAMPLES IRRADIATED IN VANDELLÓS-II REACTOR CORE
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International Conference on Nuclear Criticality (ICNC 2011)
Edinburgh, Scotland, UK, September 19-23, 2011
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2. Activation and source term calculation

2.3 Applications: Burnup Credit (ICNC-2011, ANS-2011 and Annals-paper)

part I — a journey within the reactor core

- The **host assembly** of WRZ0058 **changed its position** in the layout **every single cycle**
- **Rod** WZR0058 remained **at the periphery** of the host assembly **from 7th to 10th**
- Placed near the center of a **different assembly** all **11th** cycle long

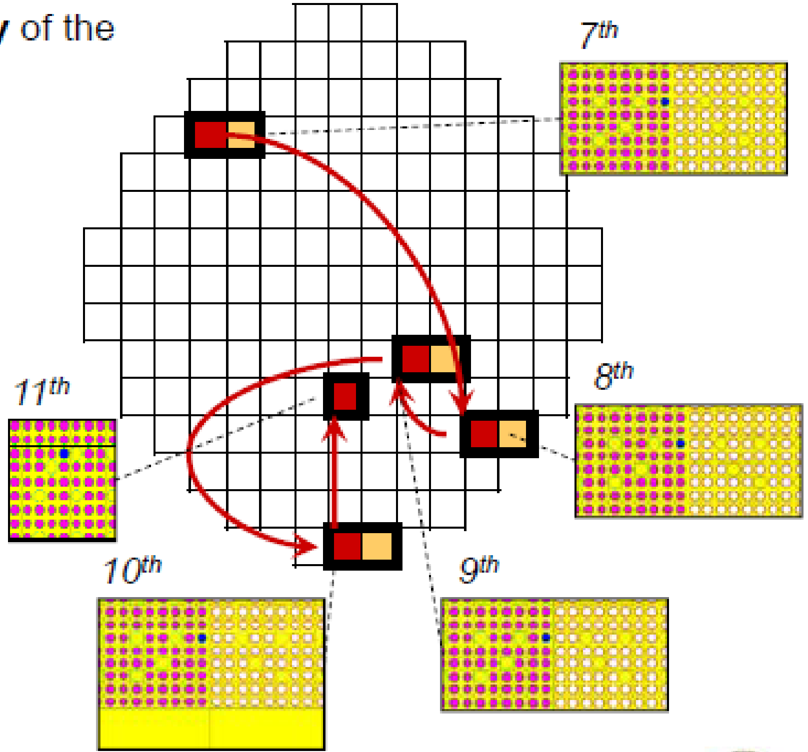
⇩

- then **it is mandatory to model**:

  i) the host assembly and its neighbor burnup

  ii) neighbor previous burnup if necessary

  iii) previous burnup of the assembly that hosts WZR0058 during 11th cycle



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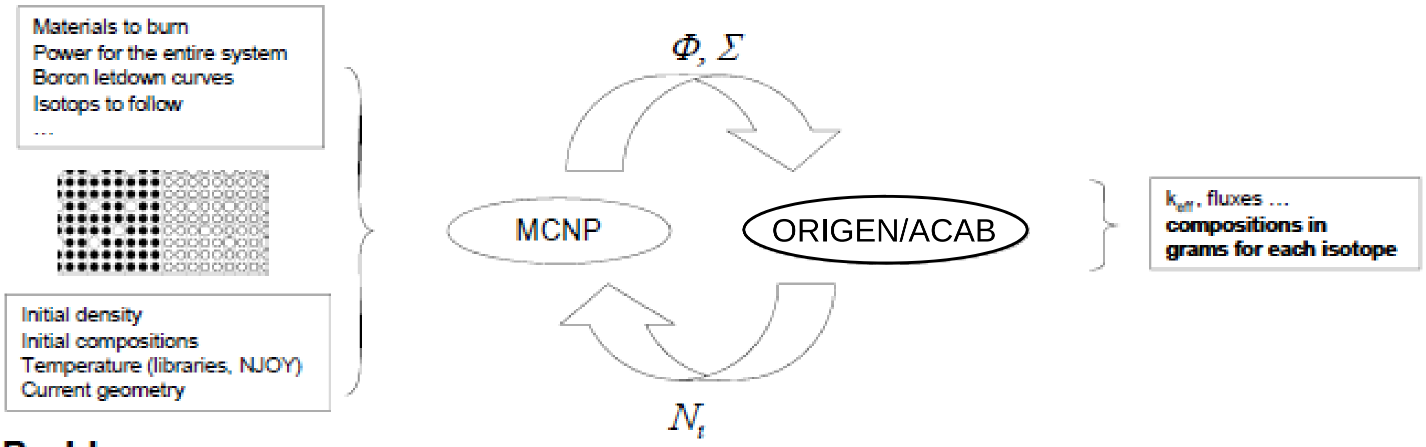
part II the LINK / [MONTEBURNS 2.0]* system

- **MONTEBURNS 2.0** couples **MCNP** and **ORIGEN2** to perform depletion calculations:



- **Problems:**

i) In each cycle, host and neighbor assemblies **inherit the resulting compositions** of previous burnup cycles

ii) MCNP **geometry changes**

→ the need of several incomplete MCNP inputs to update by hand once and again

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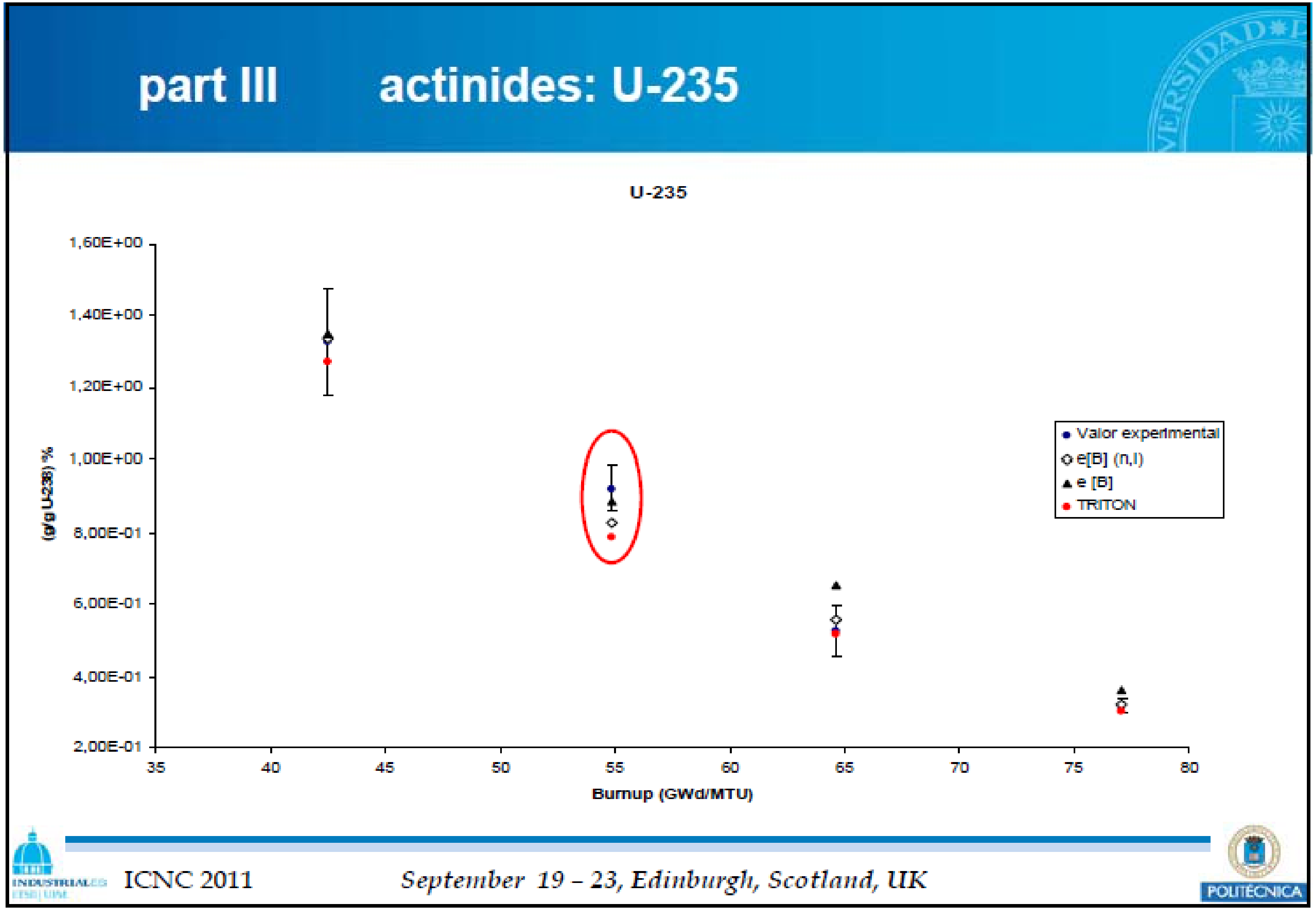

part III
actinides: U-235
U-235
1,60E+00
1,40E+00
1,20E+00
1,00E+00
8,00E-01
6,00E-01
4,00E-01
2,00E-01
(g/g U-238) %
35
40
45
50
55
60
65
70
75
80
Burnup (GWd/MTU)
Valor experimental
e[B] (n,l)
e [B]
TRITON
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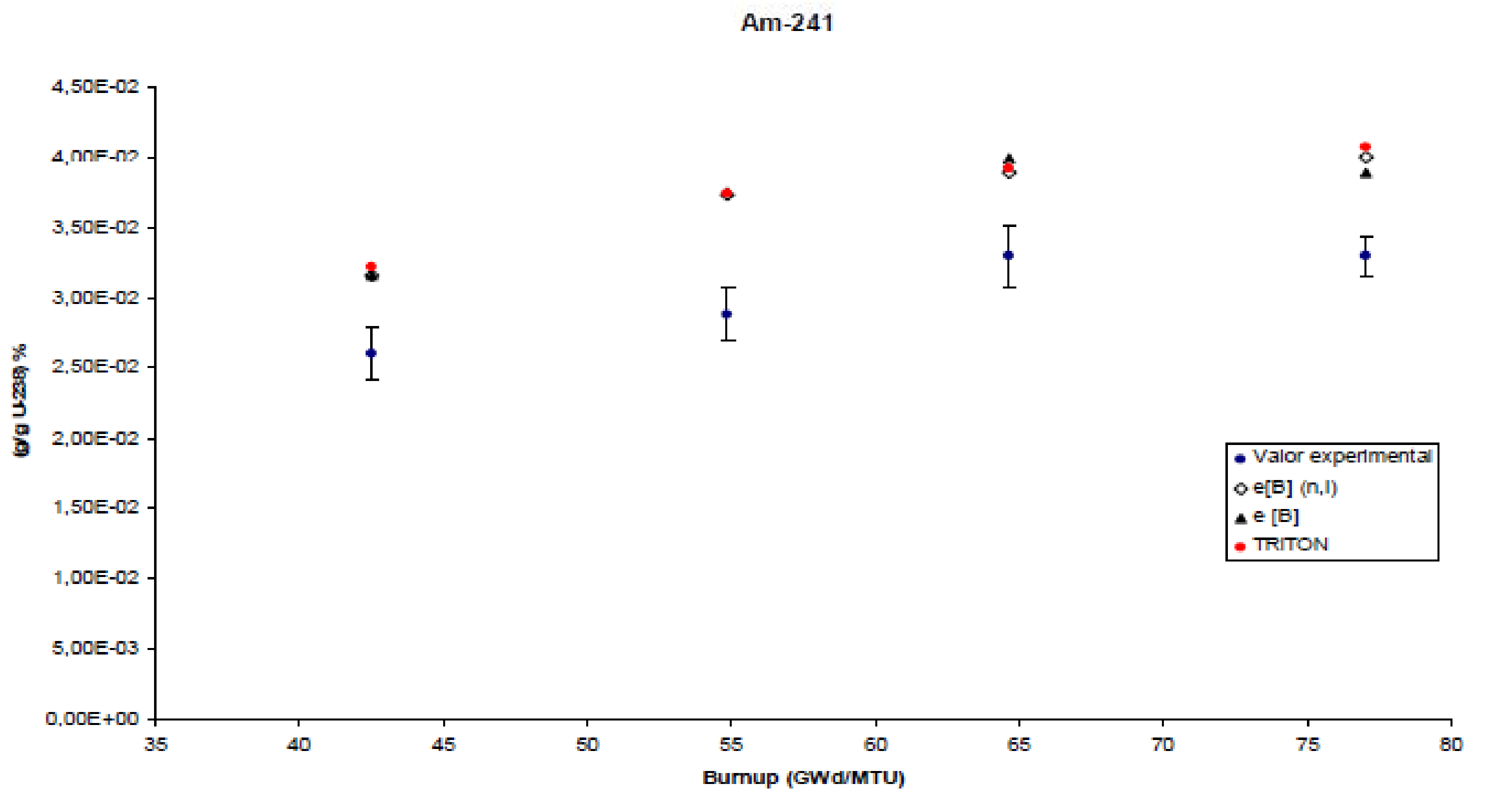
part III actinides: Am-241



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Propagation of statistical and nuclear data uncertainties in Monte Carlo burn-up calculations

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Abstract

Two methodologies to propagate the uncertainties on the nuclide inventory in combined Monte Carlo-spectrum and burn-up calculations are presented, based on sensitivity/uncertainty and random sampling techniques (uncertainty Monte Carlo method). Both enable the assessment of the impact of uncertainties in the nuclear data as well as uncertainties due to the statistical nature of the Monte Carlo neutron transport calculation. The methodologies are implemented in our MCNP–ACAB system, which combines the neutron transport code MCNP-4C and the inventory code ACAB.

A high burn-up benchmark problem is used to test the MCNP–ACAB performance in inventory predictions, with no uncertainties. A good agreement is found with the results of other participants.

This benchmark problem is also used to assess the impact of nuclear data uncertainties and statistical flux errors in high burn-up applications. A detailed calculation is performed to evaluate the effect of cross-section uncertainties in the inventory prediction, taking into account the temporal evolution of the neutron flux level and spectrum. Very large uncertainties are found at the unusually high burn-up of this exercise (800 MWd/kgHM). To compare the impact of the statistical errors in the calculated flux with respect to the cross uncertainties, a simplified problem is considered, taking a constant neutron flux level and spectrum. It is shown that, provided that the flux statistical deviations in the Monte Carlo transport calculation do not exceed a given value, the effect of the flux errors in the calculated isotopic inventory are negligible (even at very high burn-up) compared to the effect of the large cross-section uncertainties available at present in the data files.

Table 1
Summary of the main features of the code systems used by NRG

	NRG–WIMS	NRG–OCTOPUS
Transport code	WIMS8A	MCNP 4C3
Depletion code		FISPACT
Coupling algorithm		Predictor step
Burn-up steps	230	230
Cross-section libraries	JEF-2.2 based 172-group cross section library	JEFF-2.2 based point energy cross section library

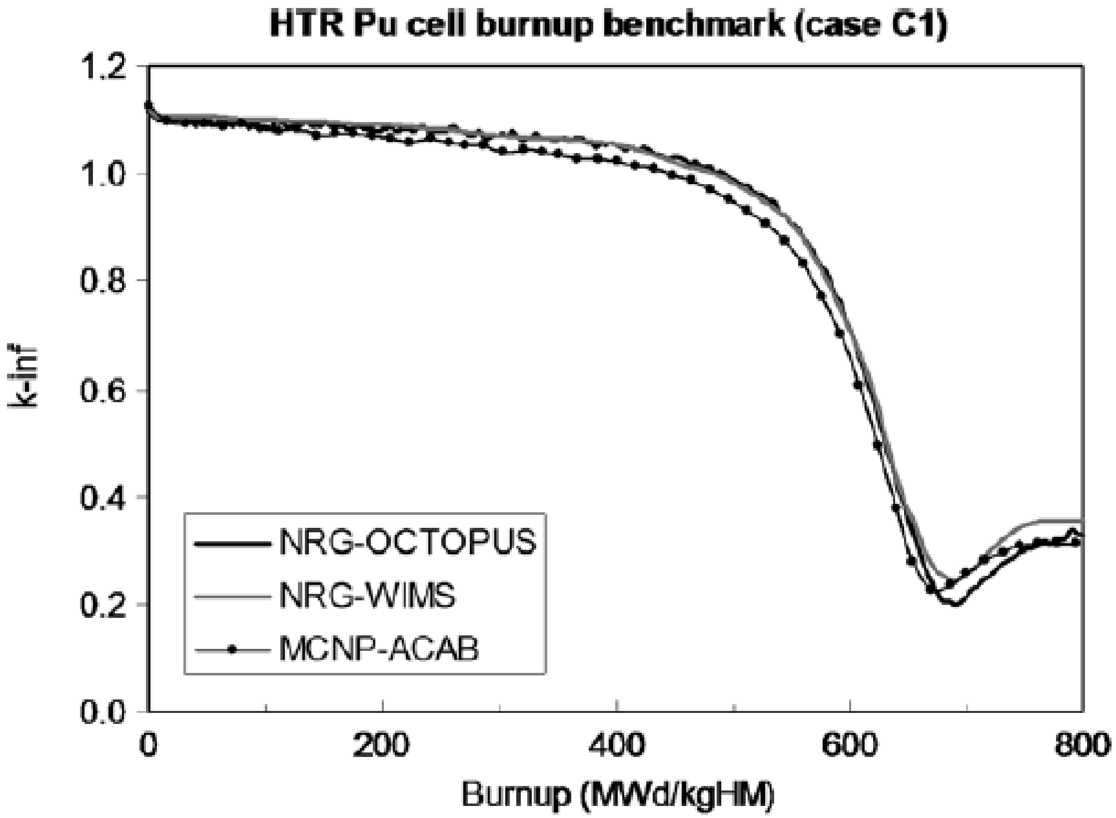

Fig. 5. Infinite multiplication factor as function of burn-up.

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Assessment of fissionable material behaviour in fission chambers

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A B S T R A C T

A comprehensive study is performed in order to assess the pertinence of fission chambers coated with different fissile materials for high neutron flux detection. Three neutron scenarios are proposed to study the fast component of a high neutron flux: (i) high neutron flux with a significant thermal contribution such as BR2, (ii) DEMO magnetic fusion reactor, and (iii) IFMIF high flux test module.

In this study, the inventory code ACAB is used to analyze the following questions: (i) impact of different deposits in fission chambers; (ii) effect of the irradiation time/burn-up on the concentration; (iii) impact of activation cross-section uncertainties on the composition of the deposit for all the range of burn-up/irradiation neutron fluences of interest. The complete set of nuclear data (decay, fission yield, activation cross-sections, and uncertainties) provided in the EAF2007 data library are used for this evaluation.

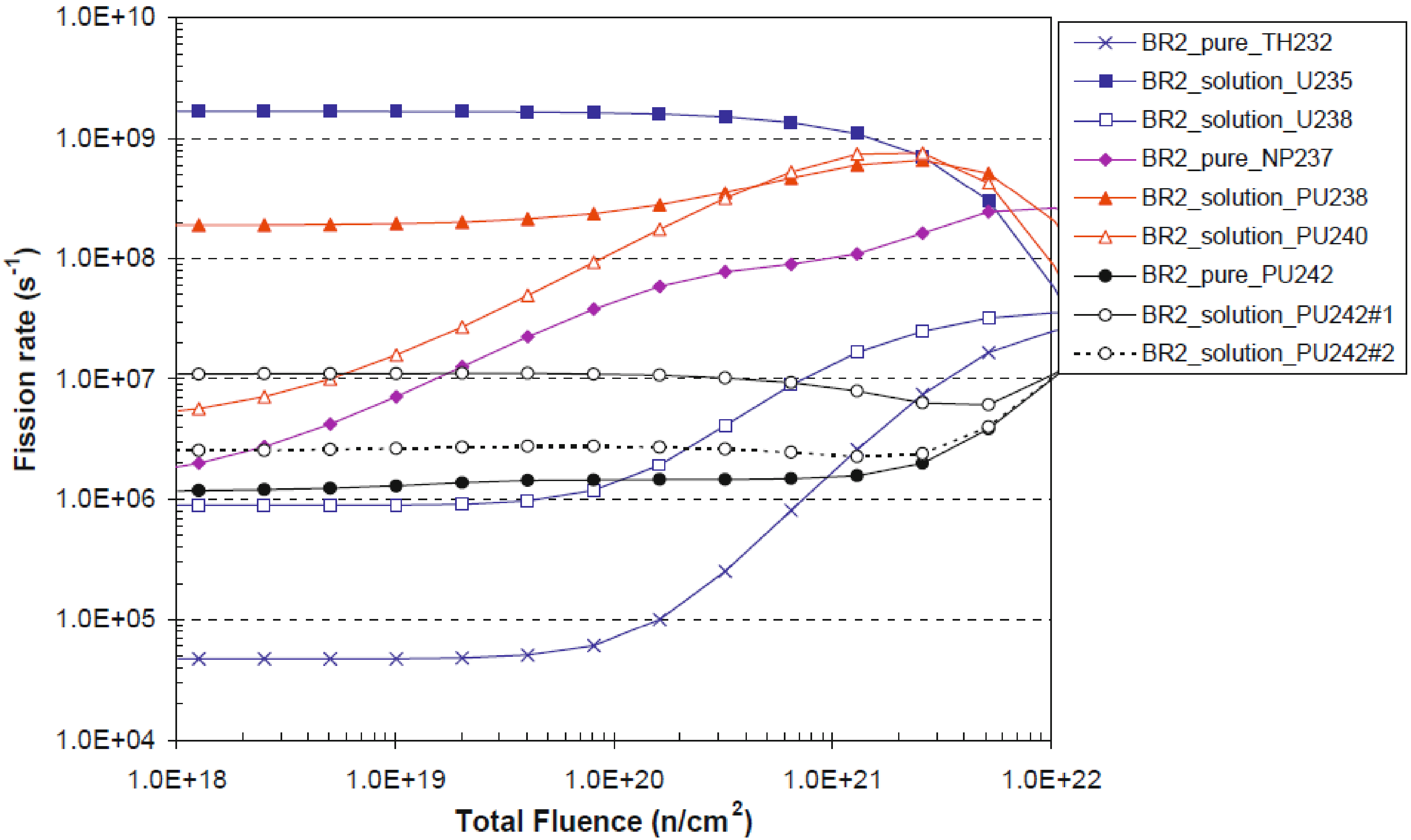

Fig. 2. Fission rates (fission/s) for the different pure and solution deposits in a typical high flux thermal neutron environment (BR2).

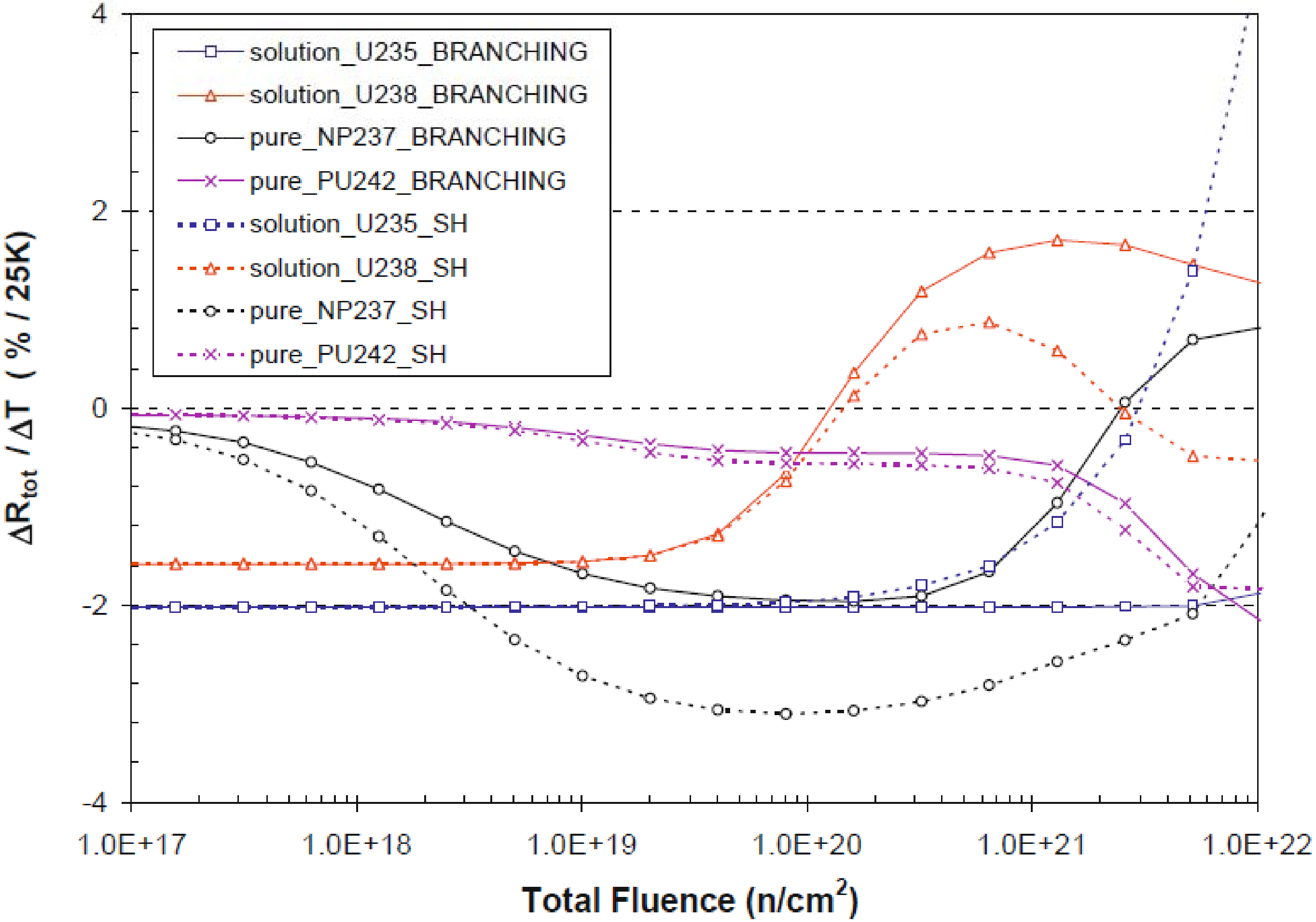

Fig. 6. Temperature dependence of the fission rates for different deposits. Branching cases show the difference in % between a reference irradiation case at 325 K and an instantaneous change in the temperature of +25 K. In the spectral history cases, we compare the nominal case at 325 K with a modified irradiation case at 350 K.

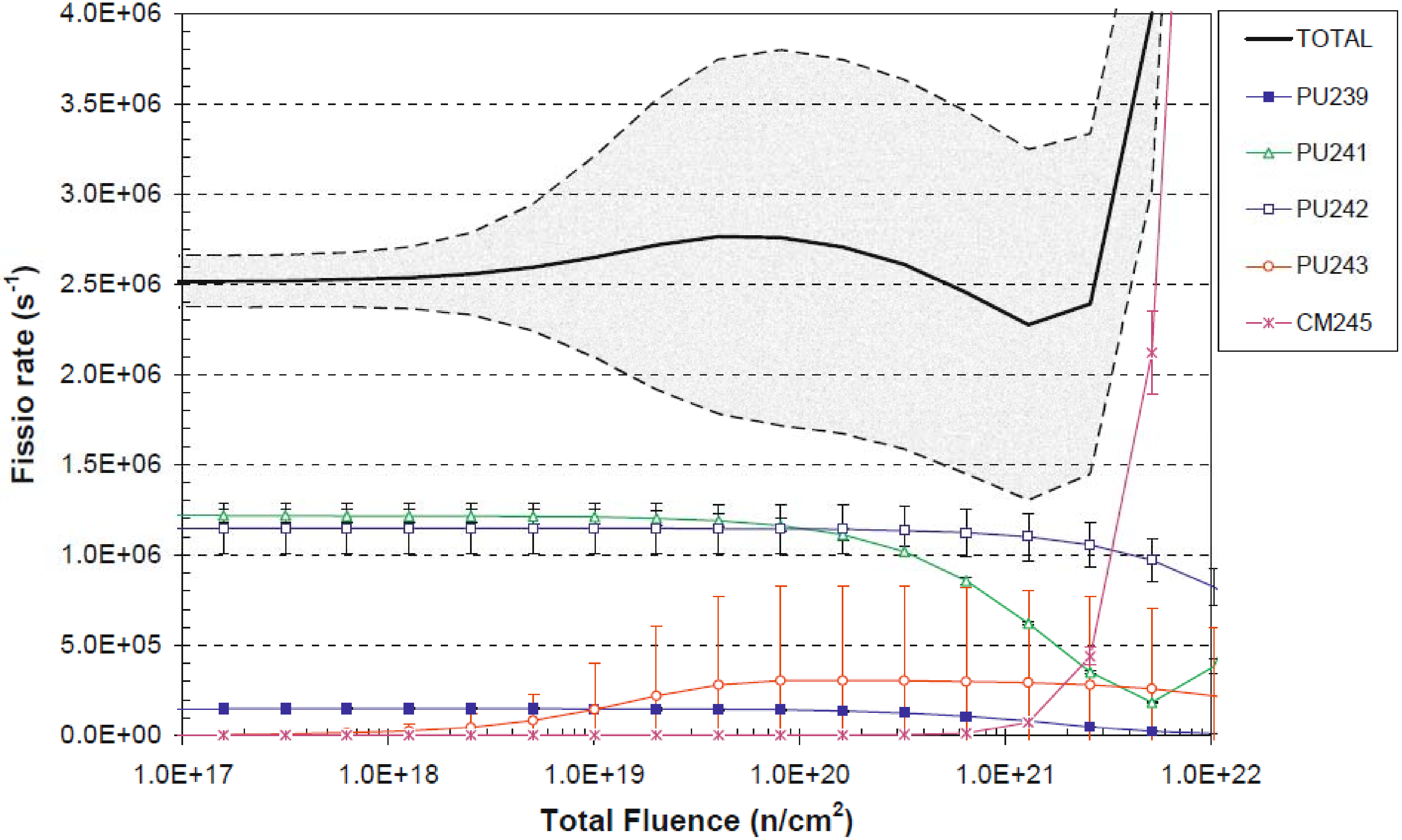

Fig. 12. Contribution and error bars (one standard deviation) of each isotope in the total fission rate for a deposit of Pu242#2 (see Table 1 for initial composition) in a typical high flux thermal neutron environment (BR2).

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Outline

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   - 1.1 Activities in JEFF: JEFF-3.1,3.11 and 3.1.2 (JEFF-May-2012)
   - 1.2 Activities in EFF : Photonuclear, DPA and STLs (EFF-Nov-2012)
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   - 3.2 Uncertainties in depletion calculation (ANS-2011)
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   - 3.6 Examples in ESFR: Uncertainty in reactivity coefficients (ND-2013)

4. Summary

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II.1. Uncertainty cross-section data

→ **From Activation-oriented nuclear data libraries**

- **FENDL UN/A-2.0, EAF2003/5/7/10-UN**

e.g.: $W^{180}(n,\gamma)$

E_{i+1}(eV)

```
W -180N,G                                                              748033102
 7.41800E+4 1.7840E+02          0          0          0              1748033102
 0.0000E+00 0.0000E+00          0        102          0              1748033102
 0.0000E+00 0.0000E+00          0          1         10              5748033102
 1.0000E-05 1.0000E+00 5.0000E+00 1.8404E-01 1.0140E+02 2.5000E-01748033102
 2.0000E+07 2.5000E-01 6.0000E+07 0.0000E+00                          748033102
```

E_i (eV)

$\Delta^2_{I=1,EAF}$ (relative error, Δ)~ $\Delta_{I=1,EXP}$= $\Delta_{I=1,EAF}/3$

Given ***V*** the G-by-G **variance matrix** of the relative cross sections vector, the variance Δ^2 of the relative spectrum-averaged cross section is: $\Delta^2 = \omega^T V \omega$

with $\omega = [\frac{\phi_1}{\bar{\phi}}\frac{\sigma_1}{\sigma^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}}\frac{\sigma_G}{\sigma^{eff}}]^T$

the total flux as $\bar{\phi} = \phi_1 + \phi_2 + \cdots + \phi_G$, and $\sigma^{eff} = \frac{\phi_1\sigma_1 + \phi_2\sigma_2 + \cdots + \phi_G\sigma_G}{\phi_1 + \phi_2 + \cdots + \phi_G}$

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II.1. Uncertainty cross-section data

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➔ General purpose ND libraries

- ENDF/B-VI.8(2001)
- ENDF/B-VIIb(2005)
- JEFF-3.0/1(2005)
- JENDL-3.3/4.0 (2010), …

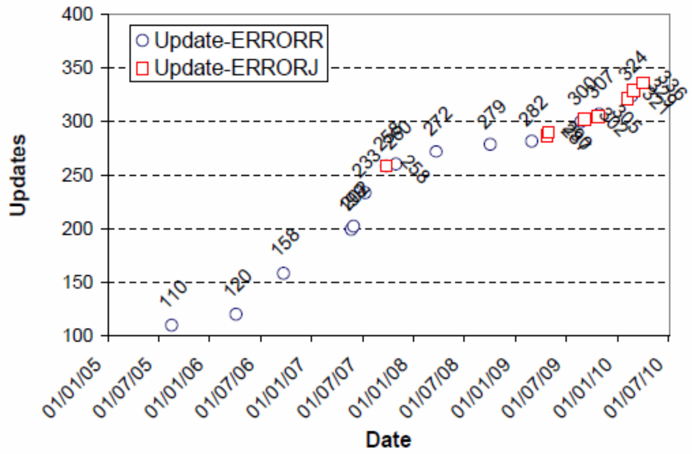
JENDL-3.3 File# 33 : Reaction Cross Section Covariance Data						
MAT	MT		Covariance with MAT, MT	MT		Covariance with MAT, MT
Pu^{239}	1 16 17 37 102	(n,Total) (n,2n) (n,3n) (n,4n) (n,g)	SELF SELF SELF SELF SELF	18	(n,fission)	SELF U^{233} (n,fission) U^{235} (n,fission) U^{238} (n,fission) Pu^{240} (n,fission) Pu^{241} (n,fission)

Future questions

covariances of isomeric data!!

radionuclide prod. yields (FILE 39)??
radionuclide prod. XSs (FILE 40) ??

- **Processing Tools (e.g. NJOY90.336)**
  - ERRORR (2005- ,14 Updates)
  - ERRORJ (2008-, 7 updates)



II.1. Uncertainty cross-section data

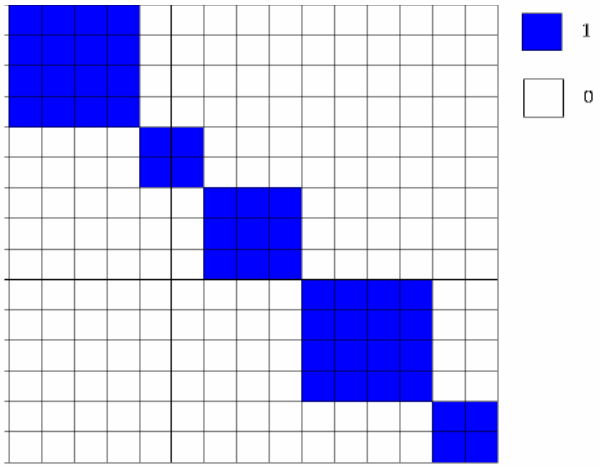
➔ "Home made" ANL covariance matrices (2005)

- G. Aliberti, G. Palmiotti, M. Salvatores, C. G. Stenberg, ***Transmutation Dedicated Systems: An assessment of Nuclear Data Uncertainty Impact***, Nucl. Sci. Eng. 146, 13-50 (2004)
- G. Palmiotti, M. Salvatores, ***Proposal for Nuclear Data Covariance Matrix***, JEFDOC 1063 Rev.1, 2005

Energy Group	MeV
1	1.96403E+1
2	6.06531E+0
3	2.23130E+0
4	1.35335E+0
5	4.97871E-1
6	1.83156E-1
7	6.73795E-2
8	2.47875E-2
9	9.11882E-3
10	2.03468E-3
11	4.53999E-4
12	2.26033E-5
13	4.00000E-6
14	5.40000E-7
15	1.00000E-7

→ set of uncertainties (diagonal values)

→ energy correlation under the form of 5 energy bands: the same for all isotopes and reactions



Data for 19 actinides (from Th-232 to Cm-245) and 3 reactions of importance: $\sigma_{(n,2n)}$, σ_{capt}, $\sigma_{fission}$

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II.2. Uncertainty decay data

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➔ Decay data

Table. Half-life and relative errors (in %) from JEFF-3.1.1 decay data library (important isotopes for ***burnup credit***)

Isótopo	$T_{1/2}$ (a)	Err(%)	Isótopo	$T_{1/2}$ (a)	Err(%)	Isótopo	$T_{1/2}$ (a)	Err(%)
C 14	5.7007E+03	0.53	I 129	1.6101E+07	4.35	U233	1.5926E+05	0.13
CL 36	3.0101E+05	1.00	CS135	2.2999E+06	13.04	U234	2.4571E+05	0.12
CA 41	1.0299E+05	3.88	CS137	3.0040E+01	0.10	U235	7.0379E+08	0.07
NI 59	7.5988E+04	6.58	SM147	1.0600E+11	1.89	U236	2.3700E+07	0.84
SE 79	3.7709E+05	5.04	SM149	2.0002E+15	0.00	U238	4.4680E+09	0.07
SR 90	2.8789E+01	0.21	SM151	8.9994E+01	6.67	NP237	2.1399E+06	0.47
ZR 93	1.5299E+06	6.54	PB210	2.2159E+01	0.54	PU238	8.7713E+01	0.34
NB 93M	1.6126E+01	0.85	RA226	1.5999E+03	0.44	PU239	2.4111E+04	0.05
NB 94	1.9986E+04	12.33	RA228	5.7514E+00	0.52	PU240	6.5626E+03	0.08
MO 93	3.9990E+03	20.00	AC227	2.1773E+01	0.01	PU241	1.4329E+01	0.28
TC 99	2.1399E+05	3.74	TH229	7.3390E+03	2.18	PU242	3.7360E+05	0.29
PD107	6.4992E+06	4.61	TH230	7.5386E+04	0.40	AM241	4.3286E+02	0.16
SN126	2.2999E+05	6.09	TH232	1.4050E+10	0.43	AM242M	1.4101E+02	1.42
SB126	3.3938E-02	0.81	PA231	3.2765E+04	0.34	AM243	7.3643E+03	0.30
SB126M	3.6315E-05	1.05	U232	6.9809E+01	0.72	CM245	8.4987E+03	2.35
						CM246	4.7310E+03	3.17

Table. Sm151

$T_{1/2}$ (y)± Error (y)	Relative error (%)	N(100 y)	s_N/N (%)
8.99999E+01 ±6.00001E+00	6/90*100=6.67%	0.4629370	5.13

$$\frac{s_N}{N} \approx \frac{\lambda}{N}\left|\frac{dN}{d\lambda}\right| \cdot \frac{s_\lambda}{\lambda} = \lambda t \cdot \frac{s_\lambda}{\lambda}$$

[ANL/NDM-154]

Future questions

- **Correlations in decay data (e.g. λ, E to decay heat applications) ?**
- **Uncertainties in gamma, beta, … spectra (e.g. dose calculations) ?**

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II.3. Uncertainty fission-yield data

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➔ Effective fission-product yield

Effective fission product yield γ^{eff}, defined as the spectrum-averaged fission yield for formation of nuclei-*i* by fission in the nuclei-*j*:

$$\gamma_{j,i}^{eff} = \frac{\gamma_1^{j,i}\sigma_1^{fiss,j}\phi_1 + \ldots + \gamma_G^{j,i}\sigma_G^{fiss,j}\phi_G}{\sigma_1^{fiss,j}\phi_1 + \ldots + \sigma_G^{fiss,j}\phi_G}$$

Given ***G*** the G-by-G variance matrix of the relative fission yield vector, the variance Δ^2 of the relative spectrum-averaged fission yield is:

$$\Delta^2 = \omega^T G \omega \quad \text{with} \quad \omega = [\frac{\phi_1}{\bar{\phi}}\frac{\sigma_{1,fiss}}{\sigma_{fiss}^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}}\frac{\sigma_{G,fiss}}{\sigma_{fiss}^{eff}}]^T$$

Table. Decay heat for PWR PIE results. Calculation for PWR UOX 5% 235U enriched, irradiated to 40 GWd/tU [R. Mills, NNL]

Cooling time (Years unless stated)	FISPIN heat (kW/tUi)	Expected bias (%)	Expected uncertainty (%)	Fraction of heat from measured nuclides (%)
Shutdown	2.45E+03	0.26	93.49	7.83
3 days	1.58E+02	0.74	49.43	52.43
5	2.18E+00	-0.31	4.76	99.35
10	1.38E+00	0.50	4.79	99.31
15	1.19E+00	0.27	4.74	99.42
20	1.07E+00	0.23	4.58	99.54
25	9.74E-01	0.35	4.43	99.63
30	8.93E-01	0.62	4.31	99.71
100	3.50E-01	7.32	4.79	100.00
1000	6.48E-02	12.35	5.82	100.00
50000	3.39E-03	7.05	6.31	99.56
100000	1.26E-03	5.07	5.06	98.78
1000000	4.58E-04	-8.59	4.90	97.87

Future questions

- **Correlations in fission-yields?**
- **Low yields have very large uncertainties?**

$$PER = 25e^{-0.25\ln(Y(A))}$$

[LA-13928, 2002]

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III.1. Methodologies in activation calculations

Goal: "to analyse how ND uncertainty is transmitted to N"

$$\boxed{\frac{dN}{dt} = AN} \Rightarrow \boxed{\frac{dN(t)}{dt} = [\lambda]N + [\sigma^{eff}]\Phi N + [(\gamma\sigma_{fiss})^{eff}]\Phi N} \quad \begin{cases} N = (N_1, N_2, \ldots) \\ N_i = N_i(\sigma, \lambda, \text{fission yields}, \phi(E)) \end{cases}$$

USING PRESENT EVALUATED COVARIANCE/UNCERTAINTY DATA:

1) Sensitivity / Uncertainty Analysis (S/U)
   - Method based on the first order Taylor series to estimate uncertainty indices for each reaction cross section in a continuous irradiation scenario (**linear approximation**)

2) Monte Carlo Uncertainty Analysis (MC)
   - To treat the global effect of all cross sections uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the cross sections
   - Assignment of a Probability Density Function (PDF) to each cross section

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III.1. Generalized Sensitivity Analysis

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$$\frac{dN(t)}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\Phi N$$

We define a random vector $\boldsymbol{\alpha} = (\sigma^{eff}, \lambda, \gamma^{eff})$

<u>We assume no-correlation between</u> σ^{eff}, λ and γ^{eff}

Let be $\hat{\alpha} = (\hat{\sigma}^{eff}, \hat{\lambda}, \hat{\gamma}^{eff})$ the best-estimated ND vector

Then, the first order Taylor series provides a means of approximating **N**$(\sigma^{eff}, \lambda, \gamma^{eff})$ about $\hat{\alpha}$

Let ***S*** be the M-by-R matrix containing the sensitivity coefficients (ρ^{ij}): $\rho_{ij} = \frac{\hat{\alpha}_j}{\hat{N}_i}\left[\frac{\partial N_i}{\partial \alpha_j}\right]_{\hat{\alpha}}$

The relative error (**e**) in the concentrations of the M nuclides is defined: $\approx$ ***S*** ε, where $\varepsilon = (\boldsymbol{\alpha} - \hat{\alpha})/\hat{\alpha}$

The variance of the relative error of concentrations : var(**e**)$\approx$ ***S* [COV ε] *S*^{T}** ***(sandwich formula)***

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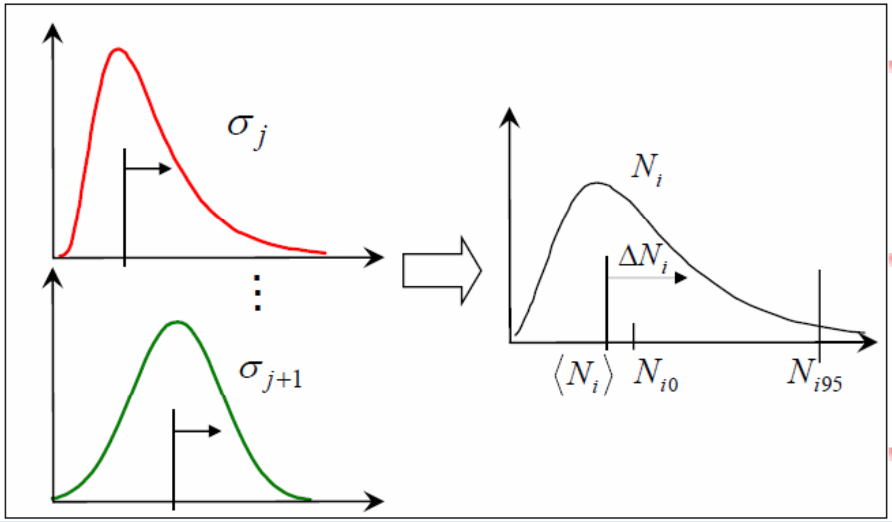
III.1. Monte Carlo method (only cross-sections)

- We use simultaneous random sampling of all the XS PDFs involved in the problem. PDF is assigned to each σ_j: $\sigma_j \to N(\sigma_{j0}, \mathrm{var}(\sigma_j)) \Longrightarrow \varepsilon_j \to N(0, \Delta_j^2)$

  $\Rightarrow$ For large values of Δ_j , σ_j could be negative!

$$\log\begin{pmatrix} (\sigma_1/\sigma_{10}) \\ (\sigma_2/\sigma_{20}) \\ \vdots \\ (\sigma_m/\sigma_{m0}) \end{pmatrix} \to N(0, M)$$

- PDF assumed to be lognormal: $\log(\sigma_j/\sigma_{j0}) = \log(1+\varepsilon_j) \approx \varepsilon_j \to N(0, \Delta_j^2)$



- From the sample of the random vector **σ**, $\sigma = (\sigma_1 ..., \sigma_j ..., \sigma_m)$ the matrix **A** is computed and the vector of nuclide quantities X is obtained $N = (N_1 ..., N_i ..., N_n)$
- Repeating the sequence, we obtain a sample of isotopic concentration vectors. The statistic estimators of the sample can be estimated
- Enables to investigate the global effect of the complete set of $\Delta\sigma$ on N

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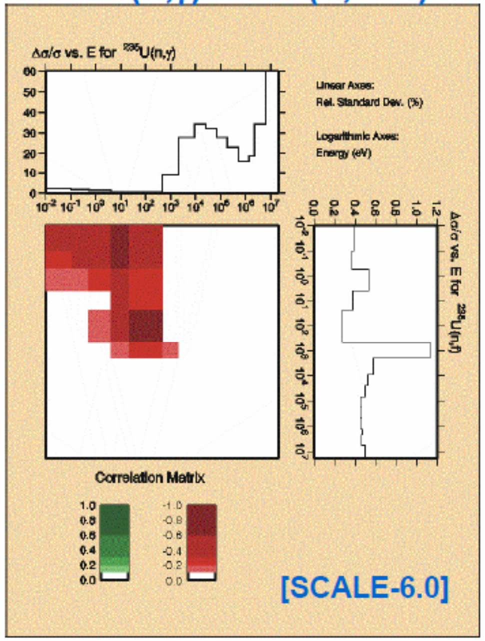
III.1. Generalized Monte Carlo method

Define a joint probability distribution of the ND errors: $\log(\alpha / \hat{\alpha}) \rightarrow N(0,V)$, where **V** is the variance matrix of the ND relative error.

Where $\alpha = (\sigma^{eff}, \lambda, \gamma^{eff})$

Correlation matrix
^{235}U (n,γ)- ^{235}U (n,fiss)



Cholesky decomposition method:

- correlations in cross sections between different isotopes and reactions (V must be definite-positive)

Letting ***P*** that verify ***V***=***PP***^{T}, it can be proven that the same **joint probability values** are obtained as follows:

- Generate $Z = (Z_1, Z_2, \ldots)^T$ independent N(0,1) random variables
- Define $Y = \boldsymbol{P} Z$, $Y = (Y_1, Y_2, \ldots)^T$
- For every random variable we estimate: $\alpha = \hat{\alpha} \cdot \exp(Y)$

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3. Sources of uncertainties in a depletion calculation

The influence of all these sources should be investigated in order to understand and quantify the uncertainties associated with computer code predictions for spent fuel isotopics:

$$\frac{dN}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\cdot \Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\cdot \Phi N = A\cdot N$$

$$N = N\left(\lambda, \sigma^{eff}, \Phi\right) = N(\lambda, \gamma, \sigma^{g}, \phi^{g}(E), \Phi)$$

- Uncertainties in decay constants: Δ_{λ}
- Uncertainties in one-group effective xs: $\Delta_{\sigma^{eff}}$

$$\sigma^{eff} = \sum_{g} \sigma^{g}\phi^{g} \Big/ \sum_{g} \phi^{g}$$

  - uncertainties in the evaluated nuclear xs data: $\Delta\sigma^{g}$
  - uncertainties in the flux spectrum obtained from the transport calculation: $\Delta\phi^{g}$
- Uncertainties in the integrated neutron flux: $\Delta\Phi$

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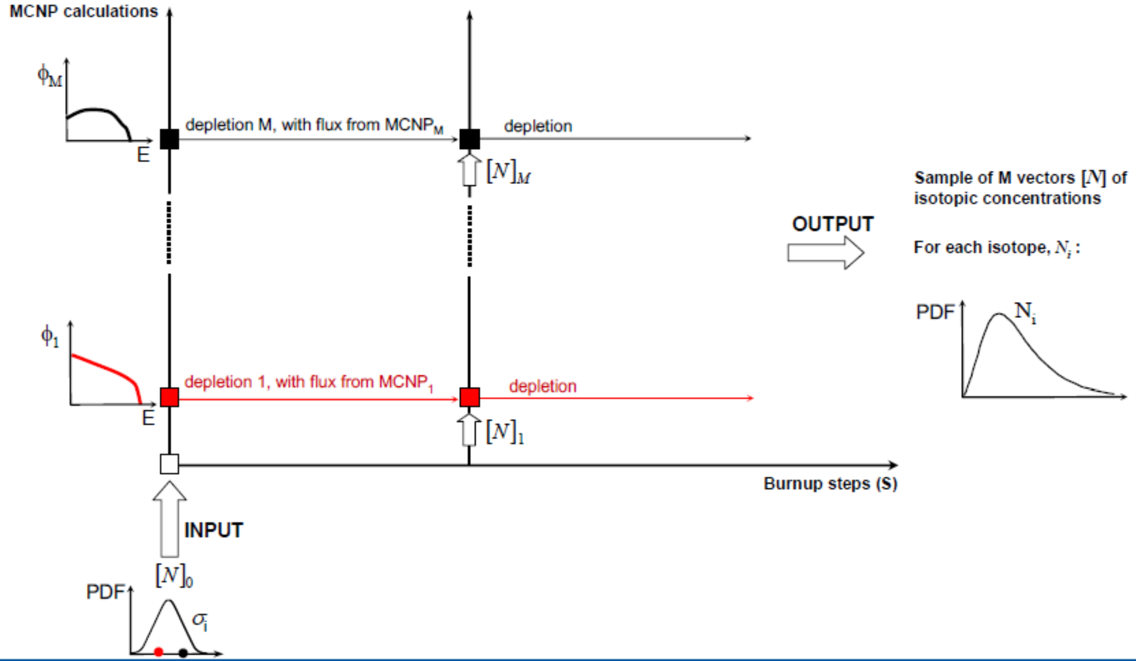
3.1 Propagation of uncertainties in burn-up calculations: "Brute Force MC"

"Brute force" random sampling method

Same sequence that the coupled calculation scheme to infer an error propagation procedure throughout the time

Simultaneous random sampling of the PDF of all the input parameters

- TMC
- NUDUNA
- XSUSA



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3.1 Propagation of uncertainties in burn-up calculations: "S/U Analysis"

Sensitivity/ Uncertainty Analysis (S/U)

Procedure based on a **first order Taylor** series approach

$$N_i(\sigma^{eff}) = N_i(\hat{\sigma}^{eff}) + \sum_{j=1}^{R} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\hat{\sigma}^{eff}} \left(\sigma_j^{eff} - \hat{\sigma}_j^{eff}\right) + \dots$$

Sensitivity coefficient ρ_{ij}

ε_j error in the 1-G effective xs

$$\sigma_j^{eff} = \sum_g \sigma_j^g \phi^g$$

$$\varepsilon_j = \sum_{g=1}^{G} \phi^g \left(\sigma_j^g - \hat{\sigma}_j^g\right) + \sum_{g=1}^{G} \sigma_j^g \left(\phi^g - \hat{\phi}^g\right) = \phi^T \boxed{\varepsilon_{\sigma_j}} + \sigma_j^T \boxed{\varepsilon_\phi}$$

errors due to uncertainties in the multigroup xs $\left[COV_{\sigma_j}\right]$

to be processed from the uncertainty libraries

errors due to uncertainties in the multigroup flux spectrum $\left[COV_{\phi}\right]$

to be obtained from a single MCNP calculation

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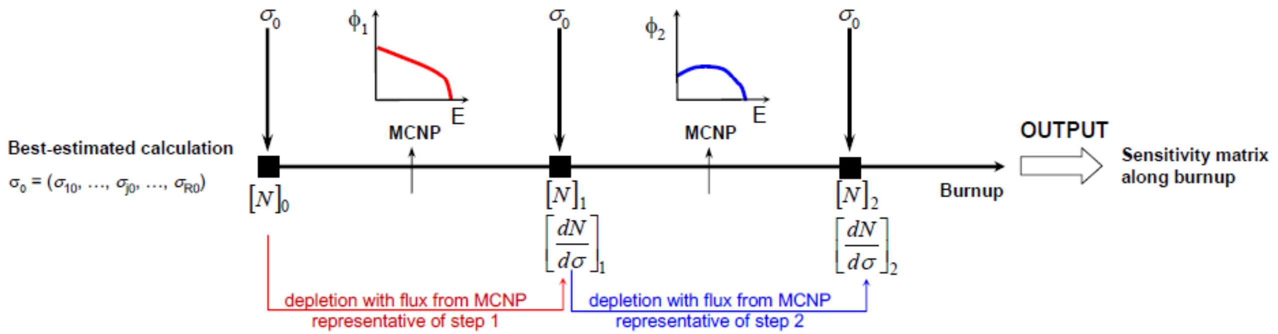
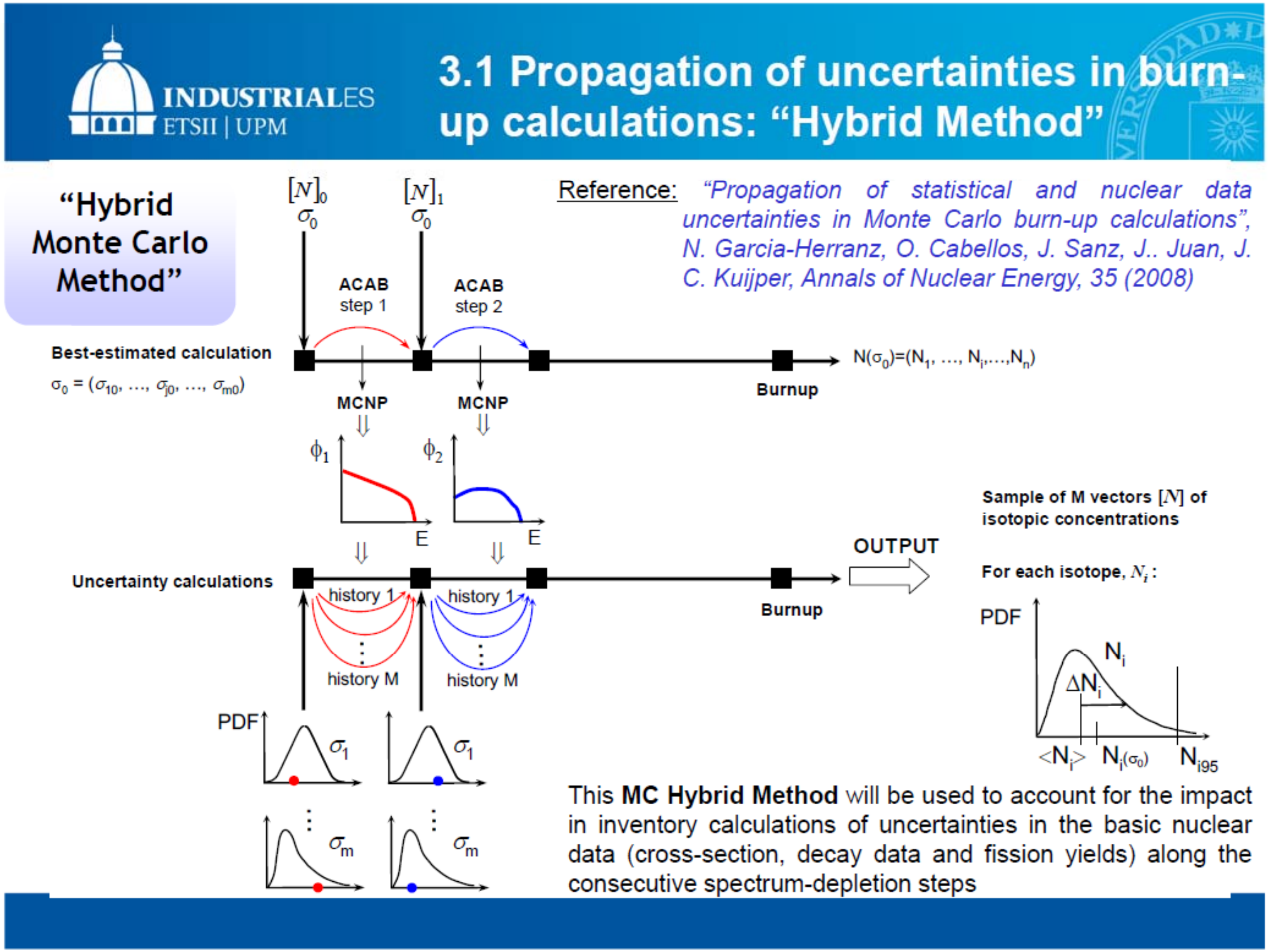
3.1 Propagation of uncertainties in burn-up calculations : "S/U Analysis"

Sensitivity/ Uncertainty Analysis (S/U)

$$N\left(\sigma^{eff}\right) - N\left(\hat{\sigma}^{eff}\right) \approx \boldsymbol{S}\,\varepsilon$$

$$var\,N \approx \boldsymbol{S}\left[COV_{\sigma^{eff}}\right]\boldsymbol{S}^{T} \approx \boldsymbol{S}\left\{ \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & & \hat{\phi}^{T}\left[COV_{\sigma_j}\right]\hat{\phi} & \\ & & & \ddots \end{bmatrix}}_{\text{Propagates the multigroup xs uncertainties when there is no statistical flux errors}} + \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & & \hat{\sigma}_j^{\,T}\left[COV_{\phi}\right]\hat{\sigma}_j & \\ & & & \ddots \end{bmatrix}}_{\text{Propagates statistical flux errors when there is no multigroup xs covariances}} \right\} \boldsymbol{S}^{T}$$





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3.1 Propagation of uncertainties in burn-up calculations: "Hybrid Method"
"Hybrid Monte Carlo Method"
Reference: "Propagation of statistical and nuclear data uncertainties in Monte Carlo burn-up calculations", N. Garcia-Herranz, O. Cabellos, J. Sanz, J.. Juan, J. C. Kuijper, Annals of Nuclear Energy, 35 (2008)
[N]0
σ0
[N]1
σ0
ACAB
step 1
ACAB
step 2
Best-estimated calculation
σ0 = (σ10, …, σj0, …, σm0)
N(σ0)=(N1, …, Ni,…,Nn)
Burnup
MCNP
MCNP
ϕ1
ϕ2
E
E
OUTPUT
Sample of M vectors [N] of isotopic concentrations
For each isotope, Ni :
Uncertainty calculations
history 1
history M
history 1
history M
Burnup
PDF
Ni
ΔNi
<Ni>
Ni(σ0)
Ni95
PDF
σ1
σ1
σm
σm
This MC Hybrid Method will be used to account for the impact in inventory calculations of uncertainties in the basic nuclear data (cross-section, decay data and fission yields) along the consecutive spectrum-depletion steps

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6.3.1 "Hybrid Method": Criticality Uncertainty Analysis in Burnup

▶ **Criticality Uncertainty Safety Analysis: "nuclear data uncertainties"**

k_{eff} it is **explicitly** dependent on the nuclear data (e.g. cross-sections, nu-bar, …) and **implicity** dependent on the number densities which characterize the system.

$$\mathrm{var}\left(\frac{\Delta k}{k}\right) \approx S_k \ \mathrm{var}\left(\frac{\Delta\sigma}{\sigma}\right) S_k^T + S_N \ \mathrm{var}\left(\frac{\Delta N}{N}\right) S_N^T$$

- the first **explicitly** term ($\Delta k/\Delta\sigma$) is calculated using TSUNAMI code:
  - Sensitivity coefficients predicted by TSUNAMI
  - Nuclear data uncertainties taken from SCALE6.1/COVA
- the second **implicitly** term ($\Delta k/\Delta N$):
  - Sensitivity coefficients for isotopes are calculated using TSUNAMI
  - Isotopic uncertainties predicted by ACAB code due to uncertainties in
    - Cross-sections
    - Fission Yields
    - Decay Data

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POLITÉCNICA

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UNIVERSIDAD POLITÉCNICA DE MADRID
ESCUELA TÉCNICA SUPERIOR DE INGENIEROS INDUSTRIALES

Propagation of Nuclear Data Uncertainties in Transmutation Calculations Using ACAB Code

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International Conference on Nuclear Data
for Science and Technology, ND2010
April 26-30, 2010
Jeju Island, Korea

ND 2010 26-30 April, Jeju Island, Korea

PART I

7

Background: Our 1st publication with MC

Second IAEA Technical Meeting on Physics and Technology of Inertial Fusion Energy Targets and Chambers

San Diego, California, 17-19 June 2002

"Monte Carlo Uncertainty Analyses of Pulsed Activation in the NIF Gunite Shielding"

J. Sanz, R. Falquina, J.F. Latkowski, S. Reyes

Abstract.

The need to estimate the effect of ***activation cross section uncertainties*** *in the accuracy of isotopic inventory calculations is an issue that is drawing more and more attention. Concerning this problem, cross section uncertainty files have been made available, such as* ***FENDL UN/A-2.0****, and some calculational procedures have been proposed. We developed a method based on the* ***first order Taylor series****, which was found practical for providing the uncertainty indices associated to each of the reaction cross sections in a continuous irradiation scenario. One of the drawbacks of the method is that its application to pulsed scenarios is difficult, and the other and most important is that it is impractical to deal with the* ***synergetic/global effect of the uncertainties of the complete set of cross sections****. To overcome these limitations, we have developed a* ***Monte Carlo procedure*** *based on simultaneous random sampling of all the cross sections involved in a problem, and it has been implemented in the activation code ACAB. The main characteristics of the method are presented here.*

PART I

8

Background: Our 1st publication for ADS

International Conference on
NUCLEAR DATA
for Science & Technology

September 26-October 1, 2004
Santa Fe, New Mexico

"Sensitivity and Uncertainty Analysis to Burn-up Estimates on ADS Using ACAB Code"

O. Cabellos, J. Sanz et al.

Abstract.

*Within the scope of the **Accelerator Driven System (ADS)** concept for nuclear waste management applications, the burnup uncertainty estimates due to uncertainty in the activation cross sections (XSs) are important regarding both the safety and the efficiency of the waste burning process. We have applied both sensitivity analysis and Monte Carlo methodology to actinides burnup calculations in a lead-bismuth cooled subcritical ADS. The sensitivity analysis is used to identify the reaction XSs and the dominant chains that contribute most significantly to the uncertainty. The Monte Carlo methodology gives the burnup uncertainty estimates due to the synergetic/global effect of the complete set of XS uncertainties. These **uncertainty estimates are valuable to assess the need of any experimental or systematic re-evaluation of some uncertainty XSs** for ADS.*

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PART I Background: Our 1st paper assessing energy correl.

ND2007

International Conference on Nuclear Data for Science and Technology

"Application of Monte Carlo techniques for propagation of cross section uncertainties to actinide inventory in ADS transmuters: comparison with sensitivity analysis",

J. Sanz, J. Juan, O. Cabellos, et al.

Abstract.

A comprehensive study is performed in order to evaluate the impact of activation cross section uncertainties on the actinide composition of the irradiated fuel in representative ADS irradiation scenarios. Some of the most recent sources/compilations of uncertainty data are used, and the results obtained from them compared. The ANL covariance matrices are taken as reference data for the calculations. The complete set of cross section uncertainties provided in the EAF2005 data library are also used for comparison purposes. In this study, the inventory code ACAB is used to analyze the following questions: impact of different correlation structures using fixed uncertainties/variances; effect of the irradiation time/burn-up on the concentration uncertainties; and applicability of Monte Carlo (MC) and sensitivity-uncertainty (SU) approaches for all the range of burn-up/irradiation times of interest in ADS designs.

PART I

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Uncertainty data

Parametric correlation matrices

Significant impact of the covariances in the inventory prediction?
How much the XS uncertainty correlations can affect the actinide inventory?

Energy range divided in G groups and E_1, E_2, … E_G mean values of each group

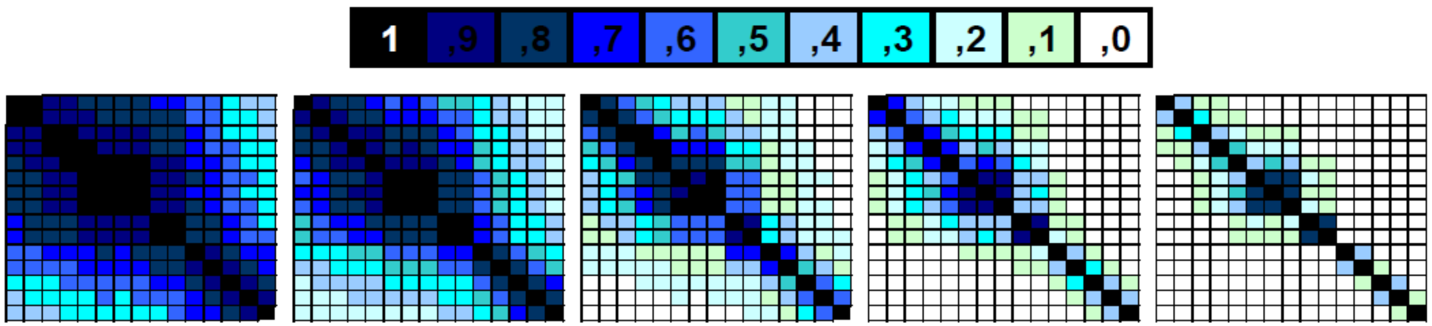
We define the correlation r_{ij} between the groups with energies E_i and E_j as :

$$r_{ij} = e^{-\theta\left|\log(E_i)-\log(E_j)\right|}$$

where θ is a positive parameter between 0 and ∞

θ small → high correlations

θ big → low correlations



$\theta = 0.05$ $\theta = 0.10$ $\theta = 0.25$ $\theta = 0.50$ $\theta = 1.0$

PART II

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Our 1st paper including overall ND uncertainties

ND2010
International Conference on Nuclear Data for Science & Technology

April 26-30, 2010
Jeju Island, Korea

ND Basic libraries used in this work

- Multigroup activation neutron cross-section basic library: EAF_N_XS-2007
- Decay data basic library: JEFF-3.1.1
- Fission yield basic library: JEFF-3.1.1

ND Uncertainty used in this work

- **Neutron cross-section** uncertainty data taken from:
  - EAF-2007/UN: the most complete set of activation uncertainties
  - SCALE6.0/COVA-44G
    - single "generic" covariance data
    - correlations for **379** materials: Light elements, FPs and actinides
    - including correlations between different isotopes and reactions
- **Decay and fission yield** uncertainty data taken and processed from JEFF-3.1.1.

Uncertainty propagation

$$\frac{dN(t)}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\Phi N$$

PART II

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II.1. Problem definition

Reference system

- One of the preliminary conceptual designs of the European Facility for Industrial Transmutation (EFIT)

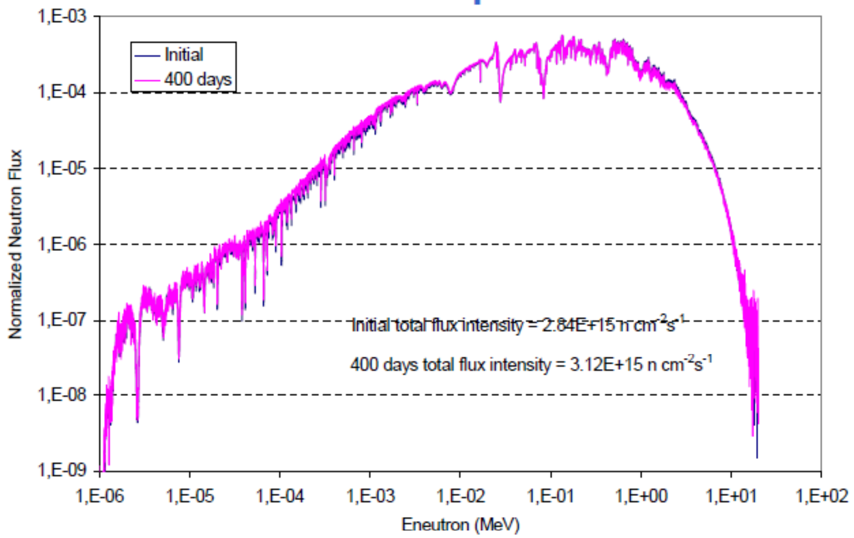
Coolant	Pure Lead
Thermal Power	400 MWth
Fuel	$(Pu, Am)O_2$ + MgO
Initial mass of actinides	2.074 tonnes

- Constant neutron environment representative of the equilibrium cycle: neutron flux: 3.12 x 10^{15} n/cm^2 s, spectrum average energy <E> = 0.37 MeV

- Calculations for discharge burn-up: 150 GWd/tHM (778 irradiation days), **corresponding to an equilibrium cycle.**

- **Assuming:**
  - Total neutron flux and ϕ(E) remain constant

Neutron flux spectrum



PART II

Uncertainty in the concentration of most relevant actinides

$^{237}Np \xrightarrow{(n,2n-M)} {}^{236M}Np \xrightarrow{\beta^-} {}^{236}Pu \xrightarrow{\alpha} {}^{232}U$ $T_{1/2}$(^{236M}Np)=1.3%, and branching error=8%)

			Uncertainty (%) due to:		
Nuclide	**N_i (#atoms)**	**N_f-N_i (#atoms)**	**λs**	**XS EAF**	**XS SCALE**
^{232}U	-	4.37E+20	5.2	9.8	1.0
^{233}U	-	1.57E+21	0.1	12.6	14.9
^{234}U	7.67E+25	6.79E+25	0.0	4.6	1.9
^{235}U	1.84E+25	1.83E+25	0.0	13.2	3.0
^{236}U	2.54E+25	2.46E+25	0.0	1.8	2.3
^{237}U	2.33E+18	4.07E+22	0.1	7.9	3.5
^{238}U	1.30E+23	1.27E+23	0.0	1.3	2.2
^{237}Np	2.25E+26	1.39E+26	0.0	6.1	1.4
^{238}Np	6.07E+18	2.40E+23	0.1	7.8	1.8
^{239}Np	2.75E+20	5.67E+20	0.2	16.3	15.9
^{238}Pu	4.26E+26	3.99E+26	0.0	4.3	2.5
^{239}Pu	5.21E+26	3.50E+26	0.0	4.8	1.3
^{240}Pu	1.73E+27	1.44E+27	0.0	1.9	0.3
^{241}Pu	3.13E+26	3.01E+26	0.0	8.3	0.9
^{242}Pu	7.50E+26	6.77E+26	0.0	2.2	0.7
^{244}Pu	1.55E+23	1.83E+23	0.0	4.0	2.2

			Uncertainty (%) due to:		
Nuclide	**N_i (#atoms)**	**N_f-N_i (#atoms)**	**λs**	**XS EAF**	**XS SCALE**
^{241}Am	3.50E+26	2.25E+26	0.0	7.0	2.0
^{242}Am	3.81E+20	1.31E+23	0.2	8.6	2.6
^{242m}Am	2.96E+25	1.81E+25	0.0	12.8	6.4
^{243}Am	3.14E+26	2.78E+26	0.0	6.1	1.4
^{242}Cm	3.17E+23	2.64E+25	0.1	10.4	3.4
^{243}Cm	3.10E+24	3.64E+24	0.2	23.4	11.7
^{244}Cm	2.67E+26	2.92E+26	0.0	6.2	3.1
^{245}Cm	7.82E+25	7.57E+25	0.0	13.2	9.7
^{246}Cm	5.20E+25	5.19E+25	0.0	7.3	3.5
^{247}Cm	1.12E+25	1.11E+25	0.0	15.7	11.0
^{248}Cm	8.33E+24	8.79E+24	0.0	6.6	4.3
^{249}Bk	-	3.28E+23	1.0	20.2	17.3
^{249}Cf	-	2.72E+23	1.1	20.4	17.9
^{250}Cf	-	8.42E+22	0.4	30.6	24.2
^{251}Cf	-	5.03E+21	0.3	44.0	30.3
^{252}Cf	-	1.03E+20	0.3	56.4	35.6

PART III

Uncertainty for FPs

This Table shows nuclides with a global uncertainty value above 6%

We assume that λ, γ and σ are not correlated:

$$\mathrm{var}(N) = \mathrm{var}(N)\big|_{\lambda} + \mathrm{var}(N)\big|_{\gamma} + \mathrm{var}(N)\big|_{\sigma}$$

Isotopes with **total** relative error > 10%

- Due to XS
  ^{94}Nb, ^{126}Sb , ^{126M}Sb, ^{150}Sm, ^{151}Sm, ^{151}Eu, 153Eu, ^{155}Gd
  ^{93}Mo (← ^{95}Mo(n,3n) with EAF rel.err 68%)

-Due to yields
  ^{126}Sb

-Due to decay data
  ^{151}Eu (← ^{151}Sm with rel.err in $T_{1/2}$=6.7%)

			Uncertainty in % due to			
Nuclide	**Ni (#atoms)**	**Nf-Ni (#atoms)**	**λs**	**γs**	**XS EAF**	**XS SCALE**
^{79}Se	-	2.25E+23	0.00	5.9	4.3	1.6
^{93M}Nb	-	1.81E+19	6.19	2.9	3.5	1.3
^{94}Nb	-	1.39E+20	0.03	5.9	17.6	4.6
^{93}Mo	-	1.45E+18	0.01	2.7	82.6	1.2
^{103}Rh	1.01E+25	4.51E+25	0.00	3.7	5.2	1.7
^{107}Pd	6.57E+24	2.86E+25	0.01	4.0	4.9	2.3
^{109}Ag	3.56E+24	1.74E+25	0.02	3.9	5.4	2.7
^{126}Sn	-	2.02E+24	0.00	7.2	4.8	2.1
^{126}Sb		2.90E+21	5.21	9.2	9.0	3.3
^{126M}Sb	-	4.43E+18	1.05	7.5	16.4	1. 9
^{129}I	-	1.06E+25	0.07	4.1	4.7	2.1
^{149}Sm	2.41E+24	7.27E+24	0.00	3.6	6. 8	4.5
^{150}Sm	1.59E+23	4.41E+24	0.01	3.0	11.0	7.7
^{151}Sm	1.47E+24	3.64E+24	0.05	4.2	10.9	6.7
^{152}Sm	1.38E+24	7.56E+24	0.01	3.1	6.6	4.0
^{151}Eu	-	3.74E+22	6.66	3.8	9.8	6.5
^{153}Eu	8.97E+23	2.75E+24	0.01	4.4	14.6	5.2
^{155}Gd	-	2.87E+23	0.26	7.1	7.8	3.8

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Sensitivity/uncertainty Analysis Applied to the Phase VII Benchmark

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PHYSOR 2010

Pittsburgh, Pennsylvania, USA
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PART I

Benchmark description

The Benchmark specifications provide (Reference: John C. Wagner and Georgeta Radulescu, *Specification for Phase VII Benchmark UO2 Fuel: Study of spent fuel compositions for long-term disposal*, NEA Expert Group on Burn-up Credit, November, 2008)

- The discharge fuel composition (4.5 initial wt% U^{235}, 50GWd/MTU)
- The cask geometry loaded with 21 PWR-UO2 17×17 fuel assemblies.

For decay calculation:

The discharge fuel composition provided contains (113 nuclides):

- Benchmark nuclides (53)
- Their relevant precursors (60)

These **Benchmark nuclides** (light element, actinide, and fission product) were selected according to:

- Its **relevance to burnup-credit** criticality calculations
- Its **contribution to radiation dose** to the public from nuclear waste repositories

For criticality calculation:

k_{eff} values are predicted for fresh fuel and isotopic compositions from the decay calculations (30 post-irradiation time steps, up to 1 000 000 years) for two cases involving:

- **Case 1**(**ACT**): a set of 11 actinides
- **Case 2** (**PFs**): a set of 14 actinides and 16 fission products

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FIG. 1. UO2 assembly geometry and guide tube locations

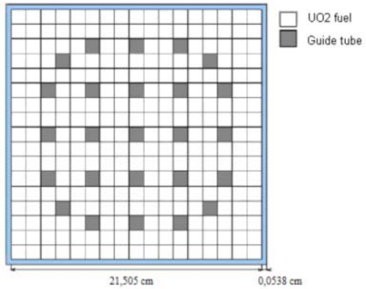
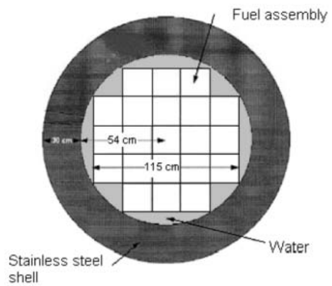


FIG. 2. Cask model (top view)



3. Uncertainty propagation

3.4 Examples in BUC: PhaseVII (PHYSOR-2010), Phase-IB (ANS-2011), High Burnup VandellosII (ICNC-2011)

PART II

2.2 Benchmark Results: Criticality calculations

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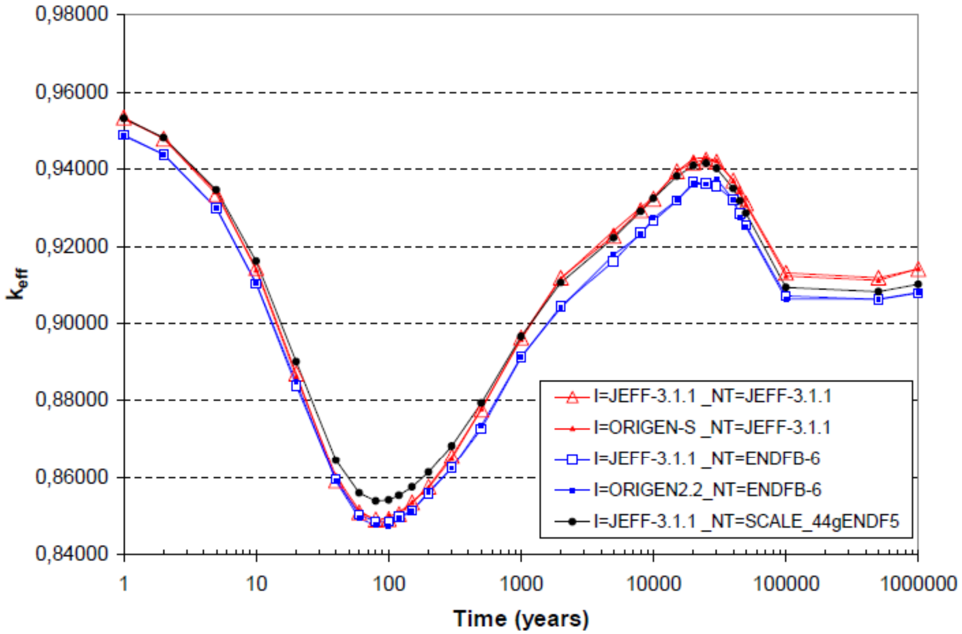
FIG 2. The calculated keff values for actinide case (**ACT**).
(I = Decay data library for the isotopic inventory; NT= Neutron transport library for keff calculation)



- k_{eff} has a maximum value at shutdown
- Minimum value at 100 years
- k_{eff} increases to another maximum around 30.000 years cooling time, this second maximum is always below the k_{eff} at shutdown

3.4 Examples in BUC: PhaseVII (PHYSOR-2010 9), Phase-IB (ANS-2011), High Burnup VandellosII (ICNC-2011)

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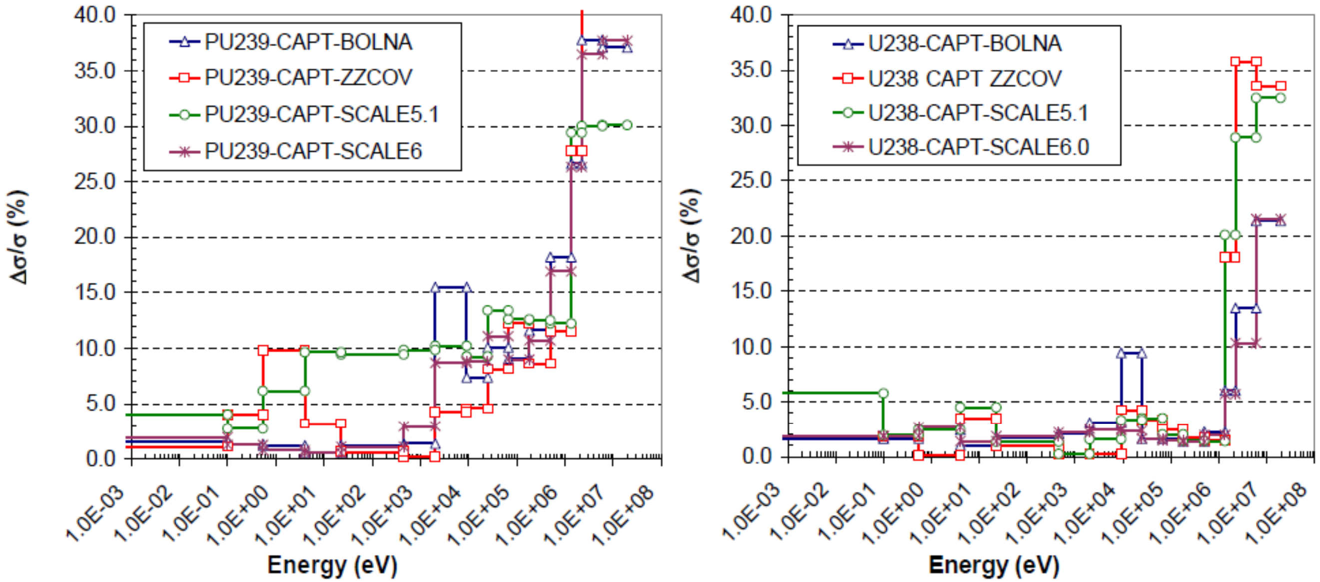
PART III

3.2.2 Error Propagation to “Criticality Calculations”: Uncertainties

FIG. 9. Relative error (%) for Pu^{239} and U^{238} capture reactions from the different source of covariance data (BOLNA, ZZ-COV, SCALE5.1 and 6.0) in a 15-groups neutron structure.



Main Conclusion: SCALE5.1 is more **conservative** than SCALE6.0 in thermal energy range

3. Uncertainty propagation

3.4 Examples in BUC: PhaseVII (PHYSOR-2010), Phase-IB (ANS-2011), High Burnup VandellosII (ICNC-2011)

PART III 3.2.2 Error Propagation to "Criticality Calculations": Results Δk_{eff}

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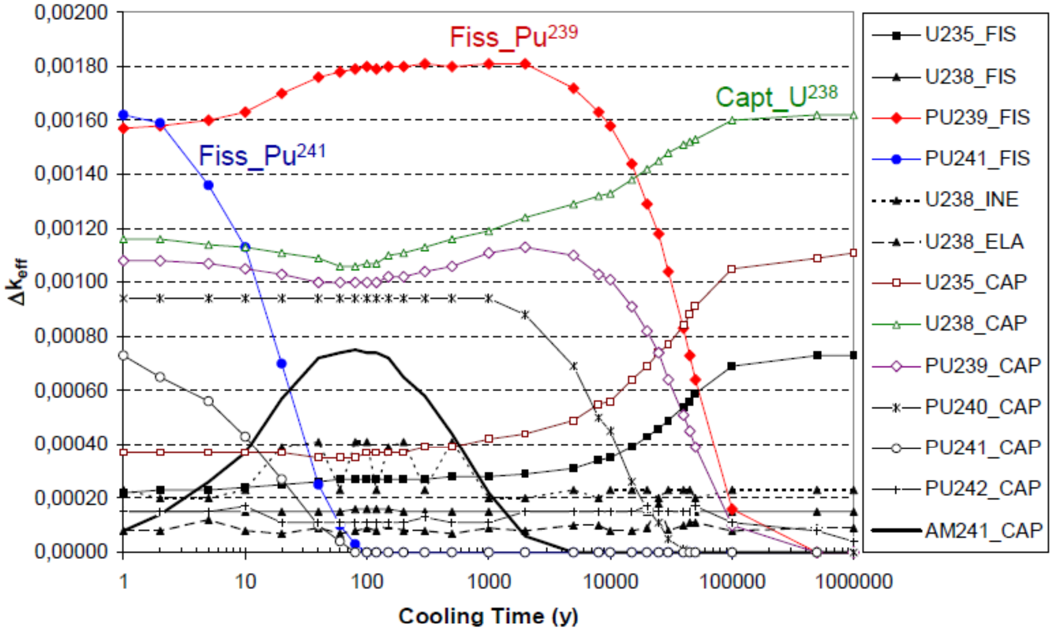
FIG. 9. Errors in keff using BOLNA diagonal uncertainty by isotope and reaction. Calculations performed for the case of actinide-only (**ACT**) burnup-credit nuclides.



Two major data sources for the overall uncertainties (> 100 pcm) are identified:

1) *Fission of Pu^{239} and Pu^{241}*
2) *Capture for U^{238}, Pu^{239}, Pu^{240} and U^{235}*

PART III 3.2.2 Error Propagation to "Criticality Calculations": Results Δk_{eff}

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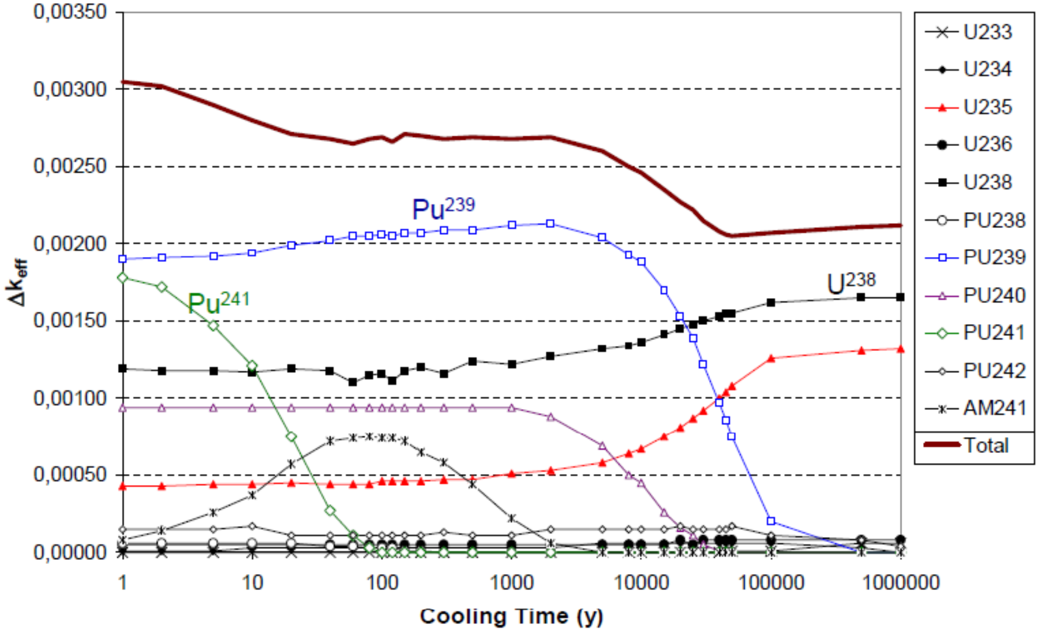
FIG. 10. Errors in keff using BOLNA diagonal uncertainty by isotope. Calculations performed for the case of actinide-only burnup-credit nuclides.

Main conclusions:

1) Relatively small uncertainties on k_{eff} are observed (< 300 pcm):

- Very small uncertainties are assumed on the low-energy data of:
  - U^{235}
  - U^{238}
  - Pu^{239}
  - Pu^{240} capture close to the first resonance

2) Significant contributions, e.g. the ^{241}Pu fission



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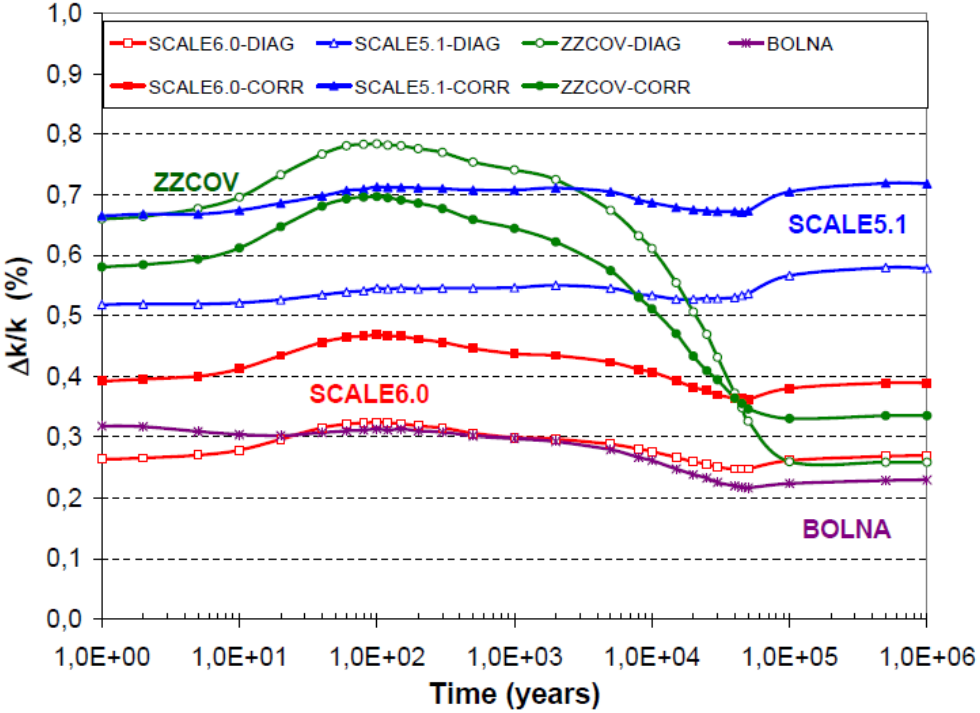
PART III

3.2.2 Error Propagation to "Criticality Calculations": Results Δk_{eff}

FIG. 11. Relative error (%) in k_{eff} values using covariance/diagonal data from ZZ-COV, SCALE5.1, SCALE6.0 and BOLNA (with only diagonal values). Calculation for actinide case.

Main conclusions:

- **Importance of energy correlations in uncertainty data!!**
  - In **BOLNA**, the maximum error is at shutdown, **~300 pcm**.
  - Using **SCALE5.1** covariance/ only diagonal values a total uncertainty of **~700/~600 pcm** is predicted.
  - With **SCALE6.0**, a total uncertainty of **~450/~300 pcm** using covariance/ only diagonal values is predicted.
  - **ZZ-COV** reaches **~700/~800 pcm** using covariance/only diagonal values at 100 years cooling time.



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ISOTOPIC UNCERTAINTY ASSESSMENT DUE TO NUCLEAR DATA UNCERTAINTIES IN HIGH-BURNUP SAMPLES

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International Conference on Nuclear Criticality
(ICNC 2011)
Edinburgh, Scotland, UK, September 19-23, 2011

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3.2 Propagation of uncertainties in burn-up calculations: "Vandellos II pin-cell"

Table I. Table I. Calculated uncertainties in actinides due to cross-section and decay data uncertainties for high-burnup.

- Uncertainties due to **cross-sections**:
  - For major actinides, the uncertainty remains below 2%. It increases for minor actinides
  - Lower uncertainties using SCALE6.0/COVA
  - Lower uncertainties for Cm isotopes using EAF2010/UN
- Uncertainties due to **decay data** remain very low, except for 243Cm with 0.4% (relative error of Cm243 half-life is 6.7%)

Isotope	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3g	EAF2010/UN 3g	SCALE6.0/COVA 44g
233U	0.1	2.5	1.9	2.1
234U	0.1	4.6	2.6	3.1
235U	0.0	1.1	1.1	0.2
236U	0.0	0.7	0.6	0.3
238U	0.0	0.3	0.3	0.1
237Np	0.0	1.3	1.5	0.7
238Pu	0.0	1.3	0.9	0.4
239Pu	0.0	1.6	1.7	0.5
240Pu	0.0	3.0	2.2	0.7
241Pu	0.0	2.1	1.6	0.5
242Pu	0.0	2.1	1.0	1.6
241Am	0.2	2.0	1.5	0.5
243Am	0.0	2.8	1.4	2.8
242Cm	0.2	2.1	1.5	0.6
243Cm	0.4	6.9	4.0	2.9
244Cm	0.1	2.5	1.1	2.1
245Cm	0.0	3.4	2.4	4.2
246Cm	0.0	4.5	1.9	2.9
247Cm	0.0	5.4	2.4	3.8
248Cm	0.0	7.4	3.0	4.0
250Cf	0.1	8.8	5.5	5.2
251Cf	0.1	9.4	6.5	6.0
252Cf	0.2	7.8	3.4	4.6

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3.2 Propagation of uncertainties in burn-up calculations: "Vandellos II pin-cell"

Table II. Calculated uncertainties in light-elements due to cross-section, fission-yields and decay data uncertainties for high-burnup.

- **Uncertainties due to decay data** remain very low, except for **151Eu - 7.3% rel. err.** (it is generated by β-decay of Sm151 with a half-life relative error of 6.7%)
- **Uncertainties due to fission yields** remain below 5%: 95Mo with 4.9% (high sensitivity to 95Zr FY) and 149Sm with 4.8% (high sensitivity to 149Pm FY)

Isotope	Fission Yields JEFF-3.1.1	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3g	EAF2010/UN 3g	SCALE6.0/COVA 44g
95Mo	4.9	0.0	0.6	0.5	0.2
99Tc	1.4	0.0	0.5	0.6	0.2
101Ru	1.8	0.0	0.5	0.5	0.3
106Ru	2.4	0.6	0.6	0.6	0.2
103Rh	1.7	0.0	4.0	1.1	0.6
109Ag	1.5	0.0	5.6	4.9	0.6
133Cs	1.1	0.0	0.7	0.4	0.5
134Cs	1.1	0.0	2.2	1.5	1.3
135Cs	1.1	0.0	1.5	1.0	0.5
137Cs	1.4	0.0	0.4	0.4	0.2
139La	1.5	0.0	0.4	0.4	0.2
140Ce	1.5	0.0	0.4	0.4	0.2
142Ce	1.4	0.0	0.4	0.4	0.2
144Ce	2.4	0.2	0.6	0.7	0.2
142Nd	1.6	0.0	2.2	1.8	1.2
143Nd	1.5	0.0	0.7	1.1	0.6
145Nd	1.5	0.0	0.7	0.5	0.5
146Nd	1.0	0.0	0.6	0.4	0.4
148Nd	1.2	0.0	0.4	0.4	0.2
150Nd	1.5	0.0	0.4	0.4	0.2

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3.2 Propagation of uncertainties in burn-up calculations: "Vandellos II pin-cell"

Table II. Calculated uncertainties in light-elements due to cross-section, fission-yields and decay data uncertainties for high-burnup.

Isotope	Fission Yields JEFF-3.1.1	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3g	Cross-section EAF2010/UN 3g	Cross-section SCALE6.0/COVA 44g
147Sm	1.7	0.0	1.8	0.6	1.7
148Sm	1.5	0.0	1.2	0.6	1.0
149Sm	4.8	0.0	13.8	3.5	6.6
150Sm	1.1	0.0	1.3	0.6	1.3
151Sm	2.8	0.2	4.0	3.0	5.0
152Sm	0.9	0.0	3.2	1.1	1.6
154Sm	1.5	0.0	0.5	0.5	0.2
151Eu	2.7	7.3	4.0	3.0	5.0
153Eu	0.9	0.0	8.6	6.0	1.2
154Eu	0.9	0.0	17.3	9.8	4.9
155Eu	1.5	0.1	29.4	9.1	7.3
154Gd	0.9	0.0	10.0	5.7	3.0
155Gd	1.5	0.2	29.1	9.0	7.2
156Gd	0.8	0.0	4.6	2.3	0.8
158Gd	1.1	0.0	9.0	1.7	1.2
160Gd	3.3	0.0	0.9	0.6	0.2

- **Higher uncertainties due to cross-section data** showing a good agreement between EAF2010/UN and SCALE6.0/COVA

- **155Gd:** it is generated by β-decay of 155Eu, with higher sensitivities to **155Eu and 153Eu (n,γ)** reactions, and 155Eu- fission yield
- **149Sm:** important contribution by β-decay of 149Pm, with higher sensitivities to **149Sm (n,γ)** reaction and 149Pm-fission yield

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3. Uncertainty propagation

3.5 Examples in criticality calculations: UAM contributions (UAM5-2011, NCSC2-2011 and UAM6-2012)

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2nd Workshop on Neutron Cross Section Covariances
Vienna University of Technology, Atominstitut

Importance of Nuclear Data Uncertainties in Criticality Calculations

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September 14 -16 2011

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2. "Cell Physics" Benchmark: Exercise I-1

To study the propagation of the uncertainty from basic data across different scale and physics phenomena → through complex coupled multi-physics and multi-scale simulations (see Ref.).

Benchmark's structure

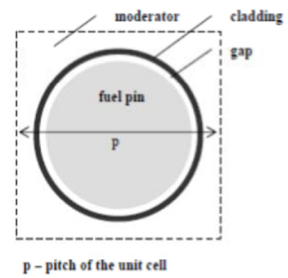
Phase I (Neutronics Phase)

- **Exercise 1 (I-1):"Cell Physics" focused on the derivation of the multi-group microscopic cross-section libraries (PWR**, BWR, VVER, GENIV …**)**
- Exercise 2 (I-2):"Lattice Physics" focused on the derivation of the few-group macroscopic cross-section libraries.
- Exercise 3 (I-3): "Core Physics" focused on the core steady state stand-alone neutronics calculations

Phase II (Core Phase)

Phase III (System Phase)

PWR (TMI-1)



4.85%wt in U235

Ref. "Verification, validation and uncertainty quantification in multi-physics modeling for nuclear reactor design and safety analysis", Maria N. Avramova, Kostadin N. Ivanov, Progress in Nuclear Energy 52 (2010) 601-614

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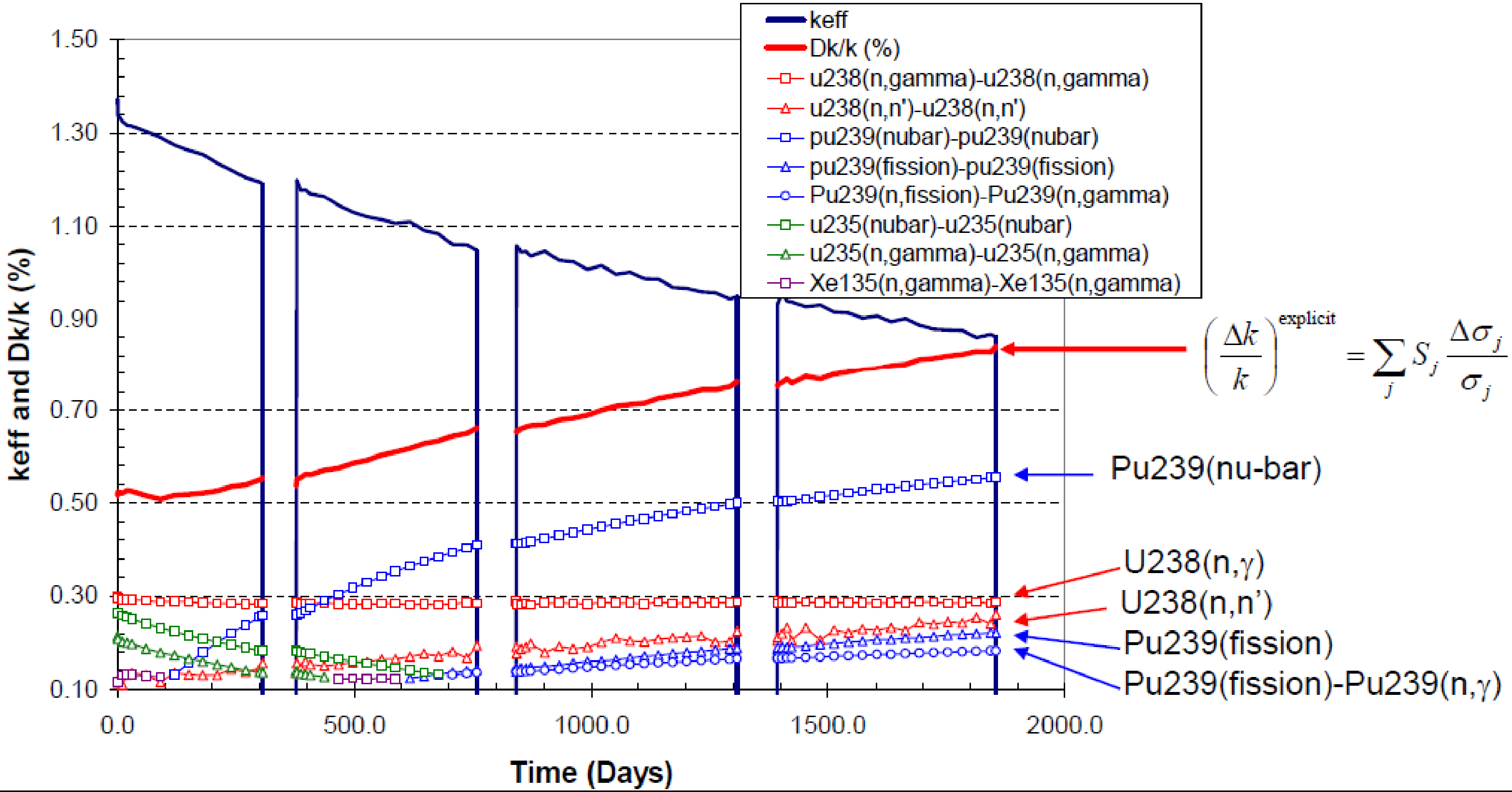
7.1 Prediction: $(\Delta k/k)^{expl}$ - SCALE/TSUNAMI

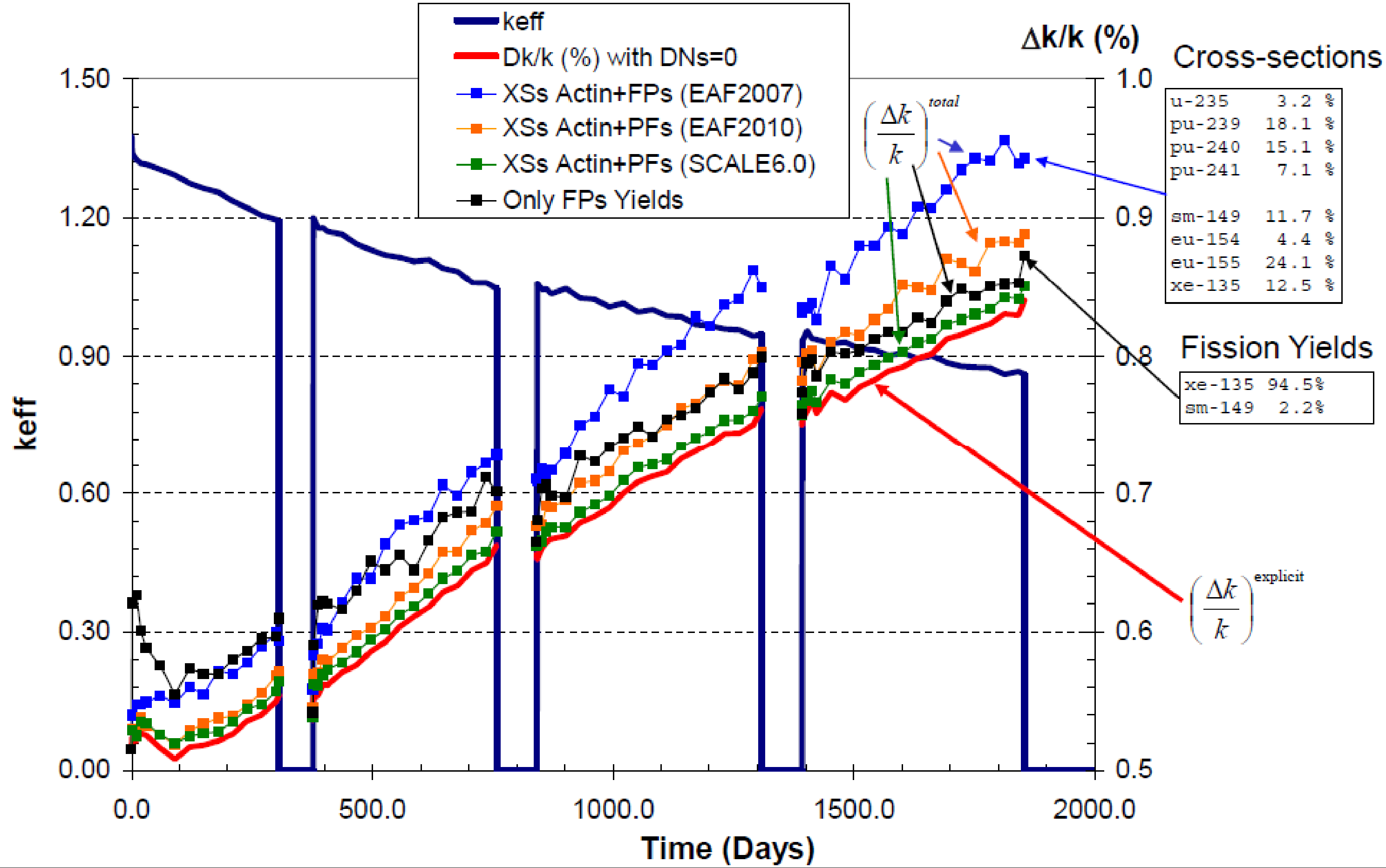
- Δk/k (%) predicted with SCALE6.0/TSUNAMI and the most important contributions
- In this figure, NO uncertainties in the isotopic inventory are taking into account!!



$$\left(\frac{\Delta k}{k}\right)^{explicit} = \sum_j S_j \frac{\Delta \sigma_j}{\sigma_j}$$

7.3 Prediction of $(\Delta k/k)^{total}$ due to $\Delta N/N$

- $\Delta k/k$ (%) due to the uncertainties in the isotopic inventory



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Presentation and discussion of submitted results for Exercise 1b: "Pin cell burnup benchmark"

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7.1 keff

	0 GWd/MTU		10 GWd/MTU		20 GWd/MTU		30 GWd/MTU		40 GWd/MTU		50 GWd/MTU		60 GWd/MTU	
	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.	mean	rel. std. dev.
GRS	1.40	0.48	1.25	0.49	1.16	0.55	1.09	0.60	1.03	0.65	0.97	0.70	0.92	0.75
XSUSA	U-238 n,gamma	0.35	U-238 n,gamma	0.29	Pu-239 nubar	0.29	Pu-239 nubar	0.39	Pu-239 nubar	0.45	Pu-239 nubar	0.49	Pu-239 nubar	0.51
	U-235 nubar	0.29	U-238 ela	0.20	U-238 n,gamma	0.19	U-238 ela	0.17	Pu-239 n,gamma	0.18	Pu-239 n,gamma	0.17	U-238 ela	0.17
	U-235 n,gamma	0.26	U-235 n,gamma	0.18	U-238 ela	0.18	Pu-239 n,gamma	0.17	Pu-239 fis	0.17	Pu-239 fis	0.17	Pu-239 n,gamma	0.16
	U-238 ela	0.17	U-235 nubar	0.17	Pu-239 n,gamma	0.14	Pu-239 fis	0.16	U-238 ela	0.16	U-238 ela	0.16	Pu-239 fis	0.16
	U-235 ela	0.13	Pu-239 nubar	0.15	Pu-239 fis	0.14	U-238 n,n'	0.12	U-238 n,n'	0.13	U-238 n,n'	0.15	U-238 n,n'	0.15
UPM	1.40	0.49	1.25	0.51	1.16	0.57	1.08	0.63	1.02	0.68	0.96	0.74	0.90	0.79
HYBRID	U-238 n,gamma	0.28	U-238 n,gamma	0.26	Pu-239 nubar	0.32	Pu-239 nubar	0.39	Pu-239 nubar	0.45	Pu-239 nubar	0.50	Pu-239 nubar	0.54
	U-235 nubar	0.26	Pu-239 nubar	0.20	U-238 n,g	0.26	U-238 n,g	0.26	U-238 n,g	0.26	U-238 n,g	0.26	U-238 n,g	0.26
	U-235 n,gamma	0.21	U-235 nubar	0.20	U-238 n,n'	0.17	U-238 n,n'	0.19	U-238 n,n'	0.21	U-238 n,n'	0.23	U-238 n,n'	0.25
	U-238 n,n'	0.12	U-235 n,gamma	0.15	u235 nubar	0.16	Pu-239 fis	0.13	Pu-239 fis	0.16	Pu-239 fis	0.19	Pu-239 fis	0.21
	U-235 n,gamma-fiss	0.10	U-238 n,n'	0.15	u235 n,g	0.12	u235 nubar	0.13	Pu-239 fis/n,g	0.15	Pu-239 fis/n,g	0.16	Pu-239 fis/n,g	0.18
	Due to Δn_XS	0.00		0.19		0.22		0.25		0.27		0.30		0.35
	Due to Δn_FYs	0.00		0.22		0.24		0.22		0.23		0.24		0.21
	Due to Δn_Decays	0.00		0.00		0.00		0.00		0.00		0.00		0.00
	TOTAL	0.49		0.58		0.65		0.71		0.77		0.83		0.89
NRG	1.41	0.68	1.25	0.79	1.16	0.78	1.08	0.76	1.02	0.76	0.96	0.76	0.90	0.79
TMC	U-235 chi	0.27	U-238 nu-bar	0.25	U-238 nu-bar	0.25	U-238 nu-bar	0.28	U-238 nu-bar	0.30	U-238 nu-bar	0.32	U-238 nu-bar	0.32
	U235-nfiss	0.24	U-235 chi	0.25	U-235 chi	0.23	Pu9-fission	0.21	Pu9-fission	0.25	Pu9-fission	0.30	Pu9-fission	0.29
	U-238-ela	0.23	U-238-ela	0.21	U-238-ela	0.20	U-235 chi	0.21	Pu9-ngamma	0.22	Pu9-ngamma	0.23	Pu9-ngamma	0.24
	U-235 n,gamma	0.22	U235-nfiss	0.21	U235-nfiss	0.19	U235-nfiss	0.18	U-235 chi	0.20	Pu9-chi	0.21	Pu9-chi	0.23
	U-238 nu-bar	0.22	U-238ngamma	0.21	U-238ngamma	0.19	Pu9-ngamma	0.18	Pu9-chi	0.17	U-235 chi	0.16	Pu9-nubar	0.15
SNU&KAERI	1.42	0.47												
	U-238 n,gamma	0.26												
	U-235 nubar	0.26												
	U-235 n,gamma	0.21												
S/U McCARD	U-238 n,n'	0.12												
	U-235 n,gamma-fiss	0.08												
	U-235 n,fiss	0.08												
	ENDFB71	0.73	--		--		--		--		--		--	0.40
	JENDL3.3	0.30												

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7.4 Number Densities

		0 GWd/MTU	10 GWd/MTU				30 GWd/MTU				60 GWd/MTU			
		mean	mean	rel. std. dev.			mean	rel. std. dev.			mean	rel. std. dev.		
				ΔXS	ΔDD	ΔFYs		ΔXS	ΔDD	ΔFYs		ΔXS	ΔDD	ΔFYs
Np-237	GRS	0.00E+00	1.69E-06	5.9			8.76E-06	3.7			2.03E-05	3.1		
	UPM	0.00E+00	1.70E-06	1.2	0.0	-	8.76E-06	0.8	0.0	-	2.03E-05	0.8	0.0	-
	NRG	0.00E+00	1.66E-06	9.5			8.84E-06	4.1			2.07E-05	2.7		
Pu-238	GRS	0.00E+00	1.23E-07	7.4			2.07E-06	4.4			1.06E-05	3.2		
	UPM	0.00E+00	1.24E-07	2.3	0.0	-	2.08E-06	1.4	0.0	-	1.07E-05	0.9	0.0	-
	NRG	0.00E+00	1.22E-07	12.1			2.15E-06	5.0			1.14E-05	2.7		
Pu-239	GRS	0.00E+00	8.07E-05	1.2			1.45E-04	1.4			1.57E-04	2.0		
	UPM	0.00E+00	8.08E-05	1.2	0.0	-	1.46E-04	1.1	0.0	-	1.60E-04	1.3	0.0	-
	NRG	0.00E+00	7.78E-05	1.8			1.40E-04	2.3			1.53E-04	3.2		
Pu-240	GRS	0.00E+00	9.36E-06	1.6			4.00E-05	1.8			7.53E-05	2.2		
	UPM	0.00E+00	9.36E-06	3.1	0.0	-	4.01E-05	2.1	0.0	-	7.59E-05	1.9	0.0	-
	NRG	0.00E+00	9.09E-06	1.9			3.89E-05	2.0			7.39E-05	2.4		
Pu-241	GRS	0.00E+00	3.55E-06	1.6			2.47E-05	1.4			4.67E-05	1.8		
	UPM	0.00E+00	3.55E-06	2.9	0.0	-	2.46E-05	1.7	0.0	-	4.68E-05	1.5	0.0	-
	NRG	0.00E+00	3.42E-06	2.0			2.42E-05	1.5			4.59E-05	2.2		
Pu-242	GRS	0.00E+00	1.98E-07	2.0			4.96E-06	2.3			2.33E-05	3.5		
	UPM	0.00E+00	1.98E-07	3.7	0.0	-	4.95E-06	1.9	0.0	-	2.31E-05	1.4	0.0	-
	NRG	0.00E+00	1.92E-07	3.0			4.98E-06	1.9			2.40E-05	1.4		

UPM: ΔN due to ΔXS, ΔFYs and ΔDD

NRG: ΔN due to ΔXS+FYs

Nuclear data uncertainty propagation to reactivity coefficients of Sodium Fast Reactor

José J. Herrero, R. Ochoa, J.S. Martínez, C.J. Díez, Nuria García-Herranz, O. Cabellos

Abstract

Engineering of new reactor models requires computational tools capable of producing results with the adequate level of accuracy. One source of uncertainty in the modeling arises from the employed nuclear data. Here, sensitivity analysis of the quantities important for safety and design to the input parameters, and posterior uncertainty propagation from the parameters to the results is a main tool to point out where nuclear data should be improved.

One such new reactor models is the **European Sodium Fast Reactor** (ESFR), and a number of such design quantities is the group of reactivity coefficients due **to heating and voiding effects**.

Here we present uncertainty propagation from nuclear data to the mentioned reactivity coefficients of the ESFR core model, with the objective of identifying the nuclear reaction data where an improvement will certainly benefit design accuracy.

ESFR full core has been modeled for SCALE6.1, and a series of steady states computed with KENO-VI Monte Carlo code using the available 238 energy groups cross sections library based on ENDFB-VII.0 based. An adjoint calculation is also performed to apply Adjoint Sensitivity Analysis Procedure (ASAP) to obtain sensitivities, first of the k_{eff} for each steady state, then for the reactivity coefficients base and perturbed states using SCALE6.1 tools. Propagated uncertainty data comes from the 44 energy groups evaluation included in the same package.

Tabla II. Valores de k_{eff} para el estado nominal

	KENO-VI 238g	KENO-VI EC	SERPENT EC
keff	1.02181 ± 0.00015	1.01731 ± 0.00010	1.01988 ± 0.00026
%Δk/k	1.7439 ± 0.0016	-	-

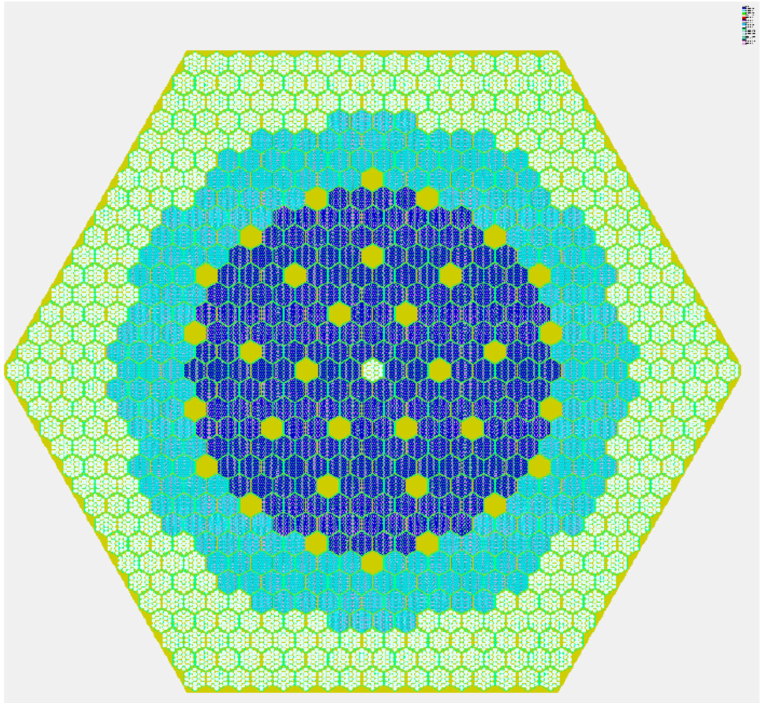

Figura 5. Corte radial del núcleo a la altura activa

Tabla III. Principales contribuyentes a la incertidumbre en k_{eff} en el estado nominal

Reacción	Contribución %Δk/k
U-238 (n,n')	1.4931E+00 ± 1.6200E-03
Pu-239 $\overline{\upsilon}$	5.5934E-01 ± 3.3883E-06
U-238 (n,γ)	3.7085E-01 ± 1.9295E-05
Pu-239 χ	3.1235E-01 ± 5.0831E-06
Pu-239 (n,γ)	2.1975E-01 ± 6.7999E-06

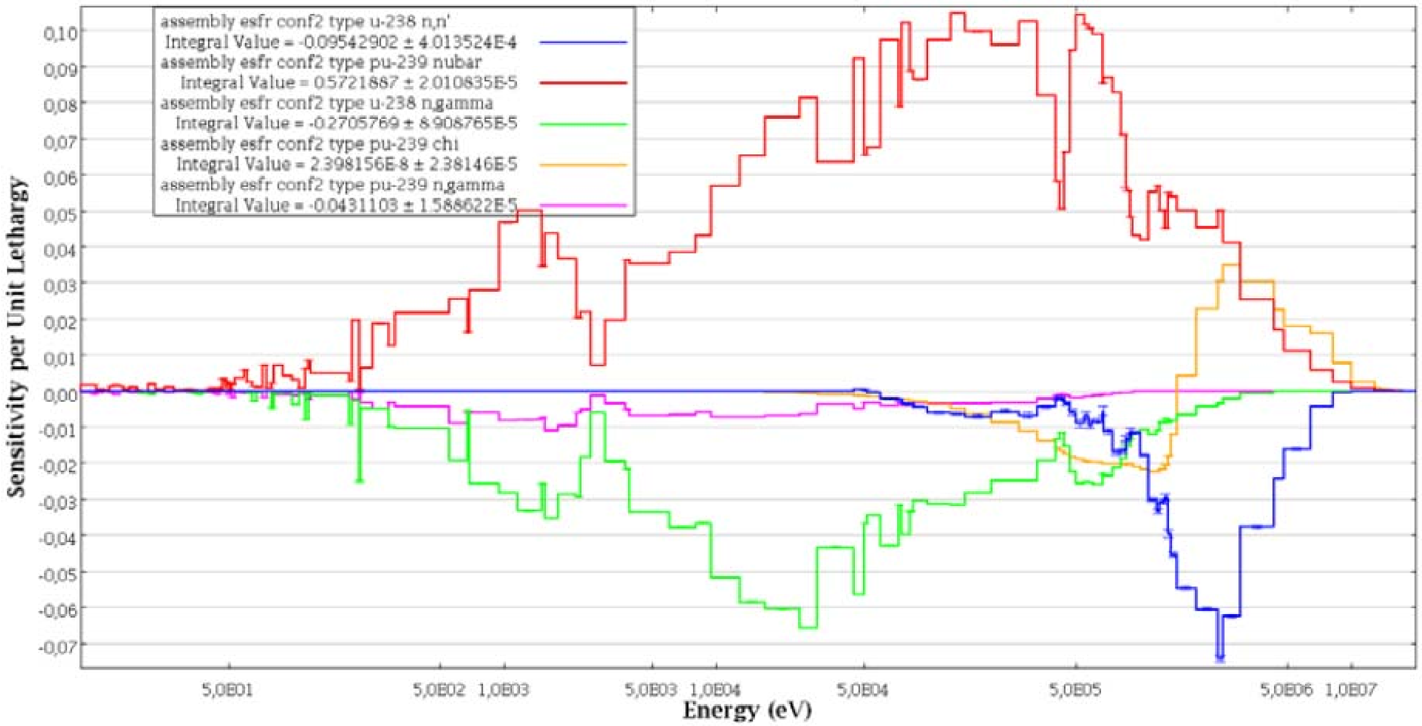

Figura 8. Sensibilidades de los 5 primeros contribuyentes a la incertidumbre en la k_{eff} del estado nominal (incluyendo barras de error no apreciables)

Tabla VIII. Reactividad introducida en el estado calentado e incertidumbre

	KENO-VI 238g	KENO-VI EC	SERPENT EC
$K_{Doppler}$ (pcm)	-977 ± 57	-1382 ± 52	-991 ± 65
$\Delta\rho$ (pcm)	-527 ± 31	-746 ± 28	-535 ± 35
Unc. $\Delta\rho$ (pcm)	30 ± 2	-	-

$$\Delta\rho = \rho_2 - \rho_1 = \frac{k_2 - k_1}{k_2 k_1}$$

$$K_{Doppler} = \frac{\rho_2 - \rho_1}{\ln\left(\frac{T_2}{T_1}\right)}$$

Tabla IX. Principales contribuyentes a la incertidumbre en la reactividad por calentamiento

Reacción	Contribución (pcm)
U-238 (n,n')	19.040 ± 1.8179
Na-23 elastic	11.657 ± 0.7392
O-16 elastic	11.554 ± 0.9192
U-238 elastic	10.261 ± 0.0126
Fe-56 elastic	6.259 ± 0.0313

Tabla X. Reactividad introducida en el estado vaciado e incertidumbre

Reactividad por vaciado			
	KENO-VI 238g	KENO-VI EC	SERPENT EC
K_{SVR} (pcm)	541 ± 32	505 ± 17	422 ± 34
$\Delta\rho$ (pcm)	541 ± 32	505 ± 17	422 ± 34
Unc. $\Delta\rho$ (pcm)	184 ± 3	-	-

Tabla XI. Principales contribuyentes a la incertidumbre en la reactividad por vaciado

Contribuciones a la incertidumbre	
Reacción	Contribución (pcm)
U-238 (n,n')	148.61 ± 2.484
Na-23 (n,n')	60.974 ± 0.0587
U-238 (n,γ)	44.611 ± 0.0340
Na-23 elastic	43.457 ± 0.2478
Pu-239 $\bar{\nu}$	40.618 ± 0.0062

$$K_{SVR} = \rho_2 - \rho_1$$

Outline

In Summary ...

LLNL

PENNSTATE

Karlsruhe Institute of Technology

NEA Nuclear Energy Agency

FUSION FOR ENERGY

CSN CONSEJO DE SEGURIDAD NUCLEAR

GOBIERNO DE ESPAÑA MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

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SCK•CEN STUDIECENTRUM VOOR KERNENERGIE CENTRE D'ETUDE DE L'ENERGIE NUCLEAIRE

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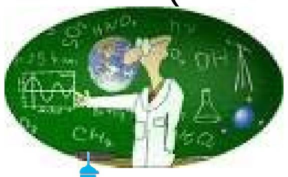

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