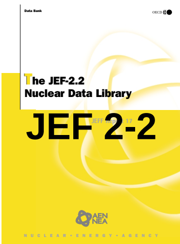

June 1993

ECN

Benchmarking of the JEF2.2 based EJ2_XMAS neutron cross-section library

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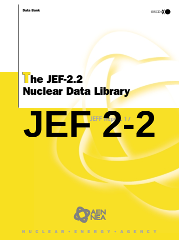
Contents

- The EJ2_XMAS library
  - Specifications
  - Remarks about JEF2.2 evaluation
- Benchmarking
  - 'Rowlands'
  - ORNL spheres
  - TRX
- Conclusions

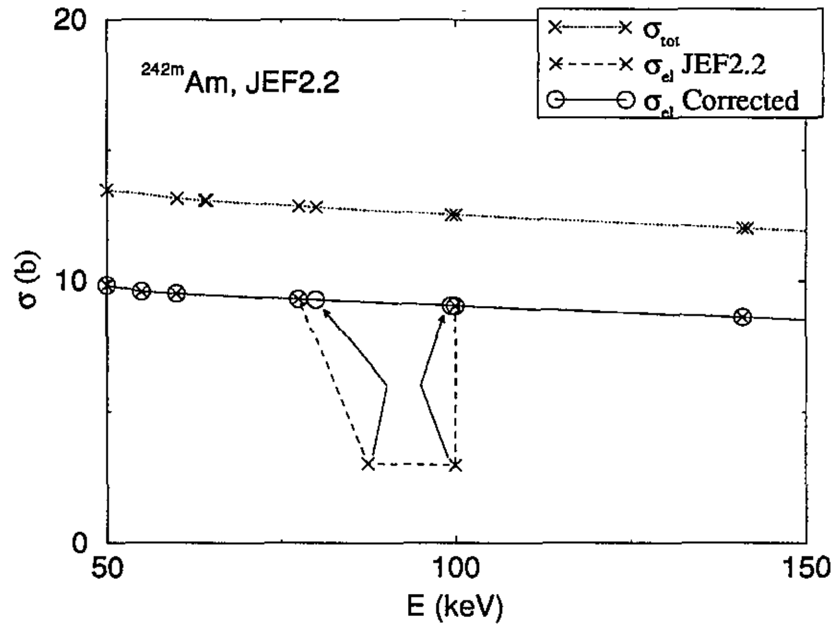
Specifications EJ2_XMAS library

- JEF2.2 based in XMAS group structure
- NJOY89.63+/NSLINK
- AMPX-M library for SCALE4.1 code system.
- Shielding: combined Nordheim/Bondarenko method for serveral T's and σ_0's if parameters given on JEF2.2.
  - Actinides: Nordheim/Bondarenko (Reich-Moore parameters converted to Breit-Wigner).
  - Structural materials with RM: Bondarenko. Other structural materials: Nordheim/Bondarenko.
  - Fission products: 20 most important Nordheim/Bondarenko. Next 20 important FP's: Bondarenko.
  - Light and heavy nuclides: Nordheim/Bondarenko.
- about 300 nuclides (6 nuclides could be processed).
- all GENDF's stored for conversion to other formats.



Remarks about JEF2.2 evaluation

1. $^{242m}_{95}$Am: Two wrong values of σ_{el} and discontinuity at 100 keV. Not all points of partials are contained in σ_t.



2. $^{230}_{92}$Th: Threshold between resolved and unresolved background (MF3) should be moved to upperlimit of resolved resonance region (from 248 eV to 251 eV; 248 eV is the energy E_0 of highest resolved resonance).

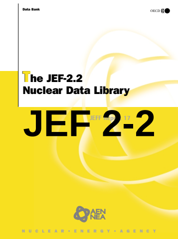
3. $^{4}_{2}$He: AWR is given in amu, should be given in amu devided by the neutron mass in amu (1.0085).

4. $^{209}_{83}$Bi, $^{239}_{93}$Np, $^{242g}_{95}$Am: contains discontinuities in σ_t.

5. $^{233}_{92}$U: large background in resolved resonance range (large self-shielding calculated with Nordheim method is incorrect).

6. Large background in unresolved resonance range for following nuclides $^{238}_{93}$Np, $^{244}_{96}$Cm, $^{249}_{97}$Bk, $^{249}_{98}$Cf, $^{253}_{98}$Cf, $^{253}_{99}$Es, $^{103}_{45}$Rh, $^{145}_{60}$Nd, $^{101}_{44}$Ru, $^{127}_{51}$I, $^{141}_{59}$Pr, $^{139}_{57}$La, $^{146}_{60}$Nd, $^{108}_{46}$Pd, $^{107}_{46}$Pd, $^{144}_{60}$Nd, ... (large self-shielding incorrect).

7. $^{58}_{27}$Co, $^{59}_{28}$Ni, $^{64}_{30}$Zn, $^{112}_{50}$Sn evaluations not complete (MF5)



Benchmark 'Rowlands' definition

Parameters of PWR Pin Cell Benchmark Model.

Region	Fuel		Clad		Moderator	
Material	UO_2		Zirconium		Water	
Outer radius (cm)	0.4		0.45		0.6770275	
CASE 1						
Temperature (K)	293		293		293	
Nuclide densities[a]	U235	7.0803E-4	Zr	4.3241E-2	H	6.6988E-2
	U238	2.2604E-2			O	3.3341E-2
	O	4.6624E-2				
CASE 2						
Temperature (K)	293		293		293	
Nuclide densities[a]	U235	7.0803E-4	Zr	4.3241E-2	H	4.6892E-2
	U238	2.2604E-2			O	2.3390E-2
	O	4.6624E-2				
CASE 3						
Temperature (K)	900		600		550	
Nuclide densities[a]	U235	7.0803E-4	Zr	4.3241E-2	H	4.6892E-2
	U238	2.2604E-2			O	2.3390E-2
	O	4.6624E-2				

[a]Nuclide densities are given in $barn^{-1}cm^{-1}$

Benchmark 'Rowlands' results

k_∞ values from CEN, AEA and ECN

Case	Fuel temperature (K)	Moderator density factor	CEN APOLLO-2 XMAS[a]	ECN PASC IJ1-XMAS[b]	AEA LWR-WIMS XMAS[c]	ECN PASC EJ2-XMAS[c]	ECN MCNP4 JEF2.2[d]
1	293	1.0	1.37905	1.38353	1.38636	1.38454	1.38952
2	293	0.7	1.32548	1.33252	1.33567	1.33431	
3	900	0.7	1.29185	1.29767	1.30322	1.30147	
Differences(pcm) †							
$2-1$			-5357	-5101	-5069	-5023	
$3-2$			-33363	-3485	-3245	-3284	
$3-1$			-8720	-8586	-8314	-8307	
Temperature coefficient $\Delta\rho/\Delta T$ $1-3$ (mN/^{0}C)			-8.1	-7.9	-7.6	-7.6	

† differences (pcm) are defined as a direct subtraction of k_∞ values multiplied by 10^5

[a] based on JEF2.0)

[b] based on JEF1.1 (IJ1-XMAS library processed by IRI, Delft)

[c] based on JEF2.2

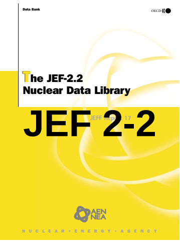
[d] MCNP library based on JEF2.2

Difference discrete ordinate method (ECN PASC) and Monte Carlo (ECN MCNP) possibly partly (about 0.2 % in k_∞) due to a too course group structure in 4 lowest energy resonances of ^{238}U in the XMAS group structure.
See paper W. de Kruijf, 'Detailed Resonance Absorption Calculations with the Monte Carlo Code MCNP and a Collission Probability Version of the Slowing Down Code ROLAIDS', to be submitted for the 'International Conference on Reactor Physics and Reactor Computations', Tel Aviv, Israel (January 1994).

Benchmark 'Rowlands' results

Neutron balance breakdown for ECN and AEA results.

	Absorption			Fission			Neutron yields		
	ECN ij1-xmas	AEA xmas	ECN ej2-xmas	ECN ij1-xmas	AEA xmas	ECN ej2-xmas	ECN ij1-xmas	AEA xmas	ECN ej2-xmas
Case 1									
H	5.606E-2	5.654E-2	5.626E-2						
O	3.563E-3	4.807E-3	4.592E-3						
Zr	7.766E-3	7.261E-3	7.309E-3						
U235	6.442E-1	6.447E-1	6.440E-1	5.344E-1	5.359E-1	5.358E-1	1.303E+0	1.307E+0	1.307E+0
U238	2.884E-1	2.867E-1	2.878E-1	2.861E-2	2.832E-2	2.773E-2	8.038E-2	7.913E-2	7.740E-2
Total	1.0	1.0	1.0	5.630E-1	5.642E-1	5.636E-1	1.383E+0	1.386E+0	1.384E+0
Case 2									
H	3.620E-2	3.658E-2	3.638E-2						
O	3.642E-3	4.901E-3	4.681E-3						
Zr	9.276E-3	8.585E-3	8.652E-3						
U235	6.163E-1	6.167E-1	6.163E-1	5.058E-1	5.077E-1	5.079E-1	1.234E+0	1.239E+0	1.239E+0
U238	3.346E-1	3.332E-1	3.340E-1	3.522E-2	3.481E-2	3.415E-2	9.881E-2	9.713E-2	9.516E-2
Total	1.0	1.0	1.0	5.411E-1	5.425E-1	5.420E-1	1.332E+0	1.336E+0	1.334E+0
Case 3									
H	3.494E-2	3.539E-2	3.510E-2						
O	3.642E-3	4.900E-3	4.681E-3						
Zr	9.151E-3	8.471E-3	8.533E-3						
U235	6.013E-1	6.012E-1	6.011E-1	4.915E-1	4.943E-1	4.944E-1	1.199E+0	1.206E+0	1.206E+0
U238	3.510E-1	3.501E-1	3.506E-1	3.523E-2	3.481E-2	3.415E-2	9.882E-2	9.713E-2	9.517E-2
Total	1.0	1.0	1.0	5.268E-1	5.291E-1	5.285E-1	1.298E+0	1.303E+0	1.301E+0



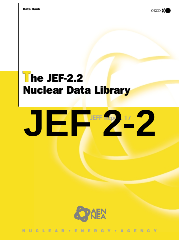
Benchmark 'Rowlands' results

Neutron balance breakdown in 6 energy groups † for ECN results

Case 1

Case 1. Absorption						
Group	H	O16	Zr	U235	U238	Total
1	1.1269E-05	4.5643E-03	2.2853E-04	2.8827E-03	3.1528E-02	3.9214E-02
2	1.2378E-05	1.2556E-08	1.6858E-04	2.4854E-03	6.6992E-03	9.3656E-03
3	3.5072E-05	2.3022E-08	3.4660E-04	2.5801E-03	1.1732E-02	1.4694E-02
4	1.8589E-03	9.8030E-07	3.5882E-03	6.3682E-02	1.5563E-01	2.2476E-01
5	9.3332E-03	4.9128E-06	5.4354E-04	9.2550E-02	1.8113E-02	1.2054E-01
6	4.5014E-02	2.1728E-05	2.4337E-03	4.7980E-01	6.4151E-02	5.9142E-01
Total	5.6265E-02	4.5919E-03	7.3091E-03	6.4398E-01	2.8785E-01	1.0000E+00
Case 1. Fission						
1				2.7521E-03	2.7689E-02	3.0441E-02
2				2.1186E-03	3.9766E-05	2.1584E-03
3				1.9543E-03	4.8010E-06	1.9591E-03
4				4.1035E-02	1.0388E-05	4.1046E-02
5				7.7064E-02	7.2398E-08	7.7064E-02
6				4.1090E-01	2.7788E-07	4.1090E-01
Total				5.3583E-01	2.7744E-02	5.6357E-01
Case 1. Neutron yields						
1				7.4266E-03	7.7258E-02	8.4684E-02
2				5.2434E-03	1.0083E-04	5.3443E-03
3				4.7708E-03	1.1959E-05	4.7827E-03
4				9.9850E-02	2.5859E-05	9.9876E-02
5				1.8796E-01	1.8022E-07	1.8796E-01
6				1.0018E+00	6.9172E-07	1.0018E+00
Total				1.3070E+00	7.7397E-02	1.3844E+00

† upper boundaries (eV): 1.96403E+07, 8.20850E+05, 1.11090E+05, 9.11882E+03, 4.00000E+00, 1.40000E-01



Benchmark 'Rowlands' results

Neutron balance breakdown in 6 energy groups † for ECN results
Case 2

Case 2. Absorption						
Group	H	O16	Zr	U235	U238	Total
1	9.9961E-06	4.6595E-03	2.8573E-04	3.5933E-03	3.8940E-02	4.7488E-02
2	1.2061E-05	1.4652E-08	2.3303E-04	3.4172E-03	9.2050E-03	1.2867E-02
3	3.4271E-05	2.6993E-08	4.8366E-04	3.6010E-03	1.6311E-02	2.0430E-02
4	1.6884E-03	1.0654E-06	4.8956E-03	8.3052E-02	1.9231E-01	2.8195E-01
5	7.7627E-03	4.8875E-06	6.4667E-04	1.0911E-01	2.1701E-02	1.3923E-01
6	2.6873E-02	1.5445E-05	2.1077E-03	4.1348E-01	5.5556E-02	4.9803E-01
Total	3.6380E-02	4.6809E-03	8.6524E-03	6.1626E-01	3.3403E-01	1.0000E+00
Case 2. Fission						
1				3.4290E-03	3.4085E-02	3.7514E-02
2				2.9121E-03	5.4010E-05	2.9661E-03
3				2.7283E-03	6.6943E-06	2.7350E-03
4				5.3767E-02	1.3884E-05	5.3781E-02
5				9.0809E-02	8.6453E-08	9.0809E-02
6				3.5423E-01	2.4066E-07	3.5423E-01
Total				5.0788E-01	3.4160E-02	5.4204E-01
Case 2. Neutron yields						
1				9.2396E-03	9.4968E-02	1.0421E-01
2				7.2064E-03	1.3695E-04	7.3434E-03
3				6.6602E-03	1.6675E-05	6.6768E-03
4				1.3083E-01	3.4564E-05	1.3086E-01
5				2.2148E-01	2.1520E-07	2.2148E-01
6				8.6363E-01	5.9909E-07	8.6363E-01
Total				1.2390E+00	9.5157E-02	1.3342E+00

† upper boundaries (eV): 1.96403E+07, 8.20850E+05, 1.11090E+05, 9.11882E+03, 4.00000E+00, 1.40000E-01

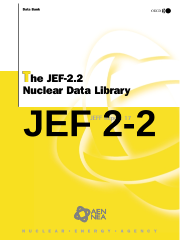
Benchmark 'Rowlands' results

Neutron balance breakdown in 6 energy groups † for ECN results

Case 3.

Case 3. Absorption						
Group	H	O16	Zr	U235	U238	Total
1	9.9958E-06	4.6595E-03	2.8571E-04	3.5935E-03	3.8942E-02	4.7491E-02
2	1.2060E-05	1.4652E-08	2.3303E-04	3.4171E-03	9.2269E-03	1.2889E-02
3	3.4259E-05	2.6983E-08	4.8345E-04	3.5997E-03	1.6633E-02	2.0750E-02
4	1.6506E-03	1.0400E-06	4.8412E-03	8.2350E-02	2.0892E-01	2.9776E-01
5	1.0469E-02	6.5741E-06	8.7102E-04	1.5485E-01	2.8170E-02	1.9437E-01
6	2.2926E-02	1.3434E-05	1.8185E-03	3.5329E-01	4.8687E-02	4.2674E-01
Total	3.5102E-02	4.6806E-03	8.5329E-03	6.0111E-01	3.5057E-01	1.0000E+00
Case 3. Fission						
1				3.4293E-03	3.4088E-02	3.7517E-02
2				2.9123E-03	5.4012E-05	2.9663E-03
3				2.7274E-03	6.6902E-06	2.7341E-03
4				5.3221E-02	1.4858E-05	5.3236E-02
5				1.2924E-01	1.1425E-07	1.2924E-01
6				3.0284E-01	2.1071E-07	3.0284E-01
Total				4.9437E-01	3.4164E-02	5.2853E-01
Case 3. Neutron yields						
1				9.2401E-03	9.4977E-02	1.0422E-01
2				7.2066E-03	1.3696E-04	7.3435E-03
3				6.6579E-03	1.6664E-05	6.6746E-03
4				1.2951E-01	3.6986E-05	1.2954E-01
5				3.1522E-01	2.8441E-07	3.1522E-01
6				7.3840E-01	5.2450E-07	7.3840E-01
Total				1.2062E+00	9.5168E-02	1.3014E+00

† upper boundaries (eV): 1.96403E+07, 8.20850E+05, 1.11090E+05, 9.11882E+03, 4.00000E+00, 1.40000E-01



Benchmark ORNL results

k_∞ values from ECN, by PASC with IJ1-XMAS, EJ2-XMAS and EJ2+O16(IJ1) libraries

Assembly		ORNL-1 H/U235 1378	ORNL-2 H/U235 1177	ORNL-3 H/U235 1033	ORNL-4 H/U235 972	ORNL-10 H/U235 1835	Average
		K_{eff}	K_{eff}	K_{eff}	K_{eff}	K_{eff}	K_{eff}
experimental values		1.00026	0.99975	0.99994	0.99924	1.00031	0.9999
ECN PASC-4	IJ1-XMAS[a]	1.00130	1.00091	0.99777	0.99919	1.00023	0.99988
	EJ2-XMAS[b]	0.99832	0.99800	0.99496	0.99641	0.99801	0.99714
	EJ2+O16(IJ1)[c]	1.00040	1.00010	0.997052	0.99851	0.999435	0.99910

[a] based on JEF1.1 (IJ1-XMAS library processed by IRI, Delft)
[b] based on JEF2.2 (EJ2-XMAS library processed by ECN)
[c] cross sections of O-16 taking from IJ1-XMAS library and the others from the EJ2-XMAS library.

Benchmark ORNL results

Neutron balance breakdown (ORNL-1) under k_{eff} calculation

	IJ1-XMAS			EJ2-XMAS			EJ2+O16(IJ1)		
	Absorption	Fission	Neutron Yield	Absorption	Fission	Neutron Yield	Absorption	Fission	Neutron Yield
H	3.311E-1			3.305E-1			3.312E-1		
N14	5.534E-4			5.524E-3			5.536E-3		
O16	2.875E-3			3.732E-3			2.835E-3		
U234	1.036E-3	9.734E-6	2.476E-5	1.037E-3	9.746E-6	2.477E-5	1.036E-3	9.757E-6	2.481E-5
U235	4.835E-1	4.109E-1	1.00125	4.821E-1	4.095E-1	0.998270	4.831E-1	4.103E-1	1.00036
U236	4.154E-5	1.165E-6	2.962E-6	4.143E-5	1.164E-6	2.958E-6	4.153E-5	1.166E-6	2.964E-6
U238	6.032E-4	7.506E-6	2.118E-5	6.006E-4	7.261E-6	2.036E-5	6.020E-4	7.273E-6	2.041E-5
Total	0.819709	0.410918	1.001299	0.823535	0.409518	0.998318	0.824351	0.4103182	1.000408

The contribution to the total absorption of ^{16}O is 0.1 % higher with JEF2.2 data than with JEF1.1
This leads to a 0.2 % lower k_{eff} with JEF2.2

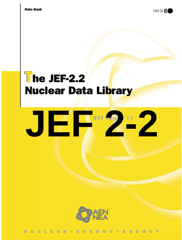
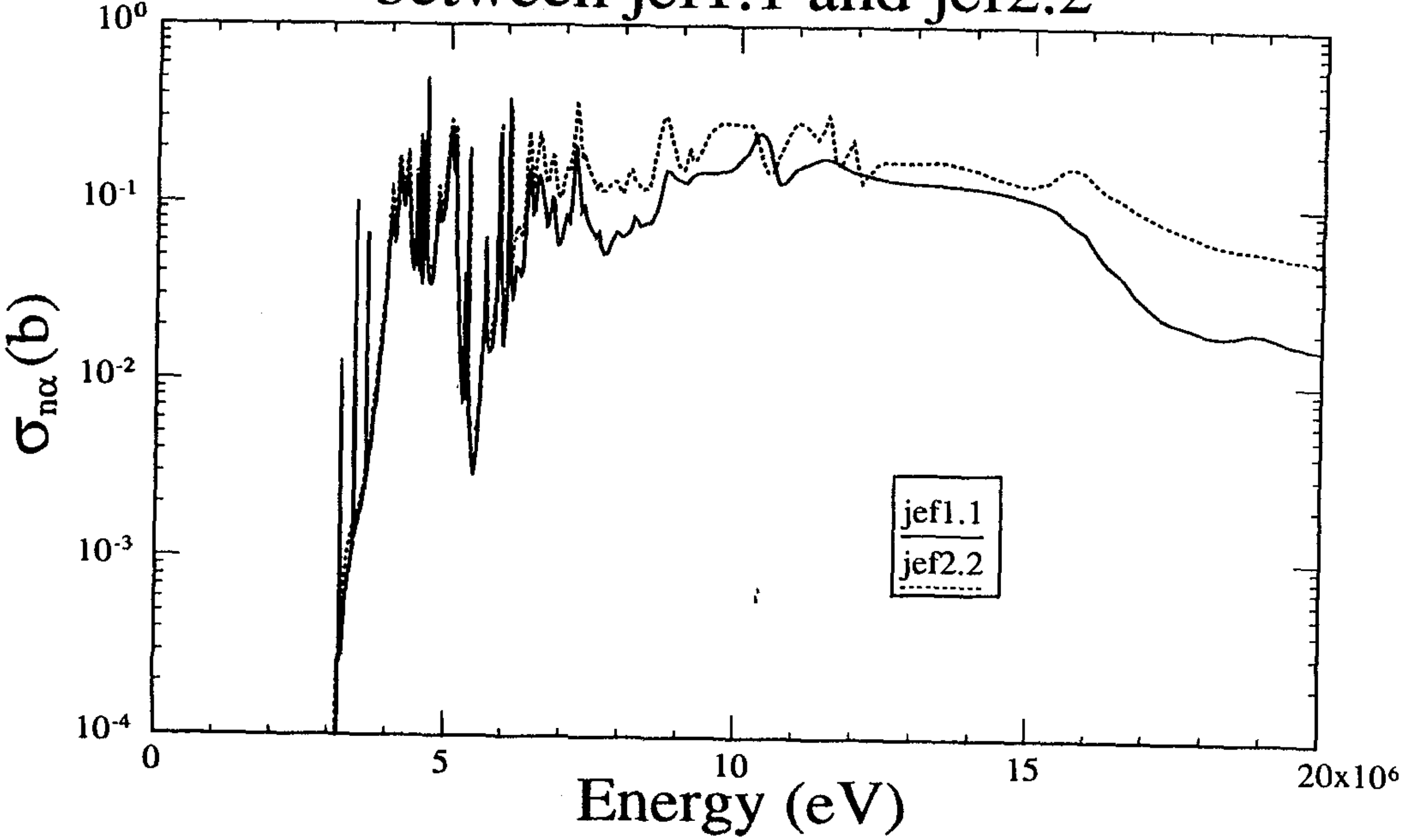
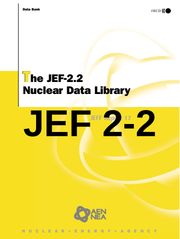


Figure 6: Comparison of $\sigma_{n\alpha}$ for ^{16}O between jef1.1 and jef2.2



TempleGraph 2.3, Origin: /home/zahir/ywang@crypton - Tue Apr 27 16:05:29 1993 (data file was j2pha)

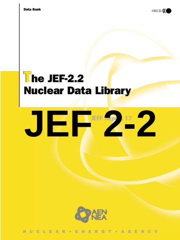


Benchmark TRX1: Preliminary results

	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C*
experiment	1.000	1.320±0.021	0.0987±0.001	0.0946±0.0041	0.797±0.008
ECN/PASC-4 with EJ2-XMAS[a]	0.9973	1.3012	0.0939	0.0941	0.7863
ECN/PASC-4 wirh IJ1-XMAS[b]	1.0001	1.3134	0.0944	0.0959	0.7864
ECN/PASC-3[c] with ECNJEF1.1[d]	0.9968	1.3266	0.0950	0.0962	0.7913
IKE[e] JEF-1	0.9960	1.3569	0.0992	0.1001	0.7984
ENDF-311[f] ENDF/B-IV	0.9876	1.3820	0.0994	0.0955	0.8060
ENDF-311 ENDF/B-V	0.9961	1.3590	0.1003	0.0983	0.7980

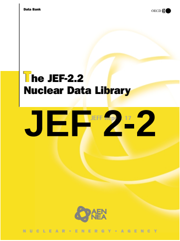
[a] based on JEF2.2 (EJ2-XMAS library processed by ECN)
[b] cross sections of O-16 taking from IJ1-XMAS library, the others taking from EJ2-XMAS library
[b] based on JEF1.1 (IJ1-XMAS library processed by IRI, Delft)
[c] J. Li et al., ECN report, NFA-LWR-92-01
[d] based on JEF1.1, 219 group library
[e] W. Bernnat et al., IKE 6-157
[f] ENDF-311, Benchmark data testing of ENDF/B-V, BNL-NCS-31531

ρ^{28} = ratio of epithermal-to-thermal ^{238}U captures
δ^{25} = ratio of epithermal-to-thermal ^{235}U fissions
δ^{28} = ratio of ^{238}U fissions to ^{235}U fissions
C* = ratio of ^{238}U captures to ^{235}U fissions



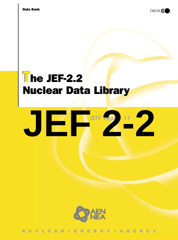
Benchmark TRX2: Preliminary results

	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C*
experiment	1.000	0.837±0.016	0.0614±0.0008	0.0693±0.0035	0.647±0.006
ECN/PASC-4 with EJ2-XMAS[a]	0.9918	0.8180	0.0580	0.0671	0.6376
ECN/PASC-4 wirh IJ1-XMAS[b]	0.9948	0.8255	0.0583	0.0685	0.6366
ECN/PASC-3[c] with ECNJEF1.1[d]	0.9923	0.833	0.0588	0.0688	0.6396
IKE[e] JEF-1	0.9973	0.8374	0.0608	0.0714	0.6393
ENDF-311[f] ENDF/B-IV	0.9935	0.863	0.0609	0.0676	0.6470
ENDF-311 ENDF/B-V	0.9984	0.846	0.0614	0.0699	0.6420



Benchmark TRX3: Preliminary results

	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C*
experiment	1.000	3.03±0.05	0.231±0.003	0.167±0.008	1.255±0.011
ECN/PASC-4 with EJ2-XMAS[a]	0.99998	2.9729	0.2264	0.1758	1.2360
ECN/PASC-4 wirh IJ1-XMAS[b]	1.0028	3.005	0.2278	0.1789	1.2409
ECN/PASC-3[c] with ECNJEF1.1[d]	0.9967	3.0486	0.2272	0.1783	1.2546
IKE[e] JEF-1	1.001	3.013	0.236	0.1725	1.2402
ENDF-311[f] ENDF/B-IV	0.9908	3.07	0.235	0.174	1.252



Benchmark TRX4: Preliminary results

	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C^*
experiment	1.000	0.481±0.011	0.0358±0.005	0.0482±0.002	0.531±0.004
ECN/PASC-4 with EJ2-XMAS[a]	0.9957	0.4764	0.0337	0.0472	0.5271
ECN/PASC-4 wirh IJ1-XMAS[b]	0.9987	0.4805	0.0338	0.0484	0.5254
ECN/PASC-3[c] with ECNJEF1.1[d]	0.9921	0.4891	0.0345	0.0491	0.5288
IKE[e] JEF-1	0.9979	0.4760	0.0344	0.0473	0.5244
ENDF-311[f] ENDF/B-IV	0.9937	0.491	0.0345	0.0467	0.5270

Conclusions

- The EJ2_XMAS library leads to satisfactory results. The results of the benchmarks are in general in good agreement with the rest of the world or the experimental results.
- The k_{eff} results of the benchmark results are in general in good agreement with the rest of the world or the experimental results but tend to be a little low.
- Special attention has to be paid to the influence of ^{16}O on the results.
- Special attention has to be paid to the discrepancy between discrete ordinate results and MCNP results.