Validation of the Pu240 Cross Section Data Available with the ERANOS Formulaire

P. Smith, G. Rimpault, O. Bouland

Introduction

The new ERANOS formulaire [1] has been developed to meet the needs of existing fast reactors as well as new evolutionary concepts such as plutonium and minor actinide burning, currently being considered in the framework of the CAPRA project. An important part of the validation and qualification of the ERANOS formulaire is the associated nuclear data and its suitability for these new reactor concepts. Several studies have shown the influence of Pu240 for the critical mass and sodium void reactivity worth of plutonium burning cores, and this paper presents the studies performed using the Pu240 cross section data available with the ERANOS formulaire. Specifically, data from the unadjusted JEF2.2 evaluation, the adjusted ERALIB1 data library [2], as well as a partial new evaluation based on measurements performed at ORNL, Hanford and Geel on the resonance region [3] have been used to determine the critical mass and the Doppler coefficient for two situations with an important quantity of Pu240: the CIRANO Plutonium Vector measurements and the CAPRA PuN core design.

Calculational Scheme

The generation of application data libraries from an evaluated nuclear data file for use with the ECCO cell code is achieved using the codes NJOY and CALENDF to produce infinite dilution cross sections, matrices and probability tables. The codes MERGE and CRECCO perform a certain number of verifications and internal consistency checks before producing a file in a format directly useable by ECCO. In this way the file ECCOLIB2 has been created containing 1968 group cross section data for the 37 most important isotopes (including Pu240) based on the unadjusted JEF2.2 data evaluation.

The development of the ERANOS formulaire for existing as well as evolutionary core designs has included the creation of an adjusted data library ERALIB1. The adjustment procedure, starting from the file ECCOLIB2, is based on coherent statistical methods and provides a rigorous technique for the reduction of the bias and uncertainty associated with nuclear data. The integral experimental data used for the adjustment includes over 300 experiments sensitive to the most important nuclear processes (production, absorption, slowing down, leakage) over a large energy range. The adjustment has been performed for the 17 most important isotopes, including Pu240. However the adjustment made to the Pu240 cross section data is based on experiments more sensitive to the upper part of the energy spectrum (> 700 KeV).

Initial calculations performed on the CAPRA PuN core design [4], where Pu240 capture dominates the Doppler effect, have shown curious non-physical behaviour associated with the temperature dependence of the cross sections, thought to be caused by the resonance structure shown in Figure 1. It can be seen that for the JEF2.2 (and therefore the ERALIB1) capture cross section of Pu240 there is an imposed background cross section which was added in order to compensate for missing resonances that effectively cuts the resonance structure. The complete resonance structure shown in Figure 1 is based on measurements performed at ORNL, Hanford and Geel. The subsequent determination in the low energy range (0-100eV)

of the variance and covariance matrices of the resonance parameters and the average cross sections for Pu240 has been performed using the Bayesian R matrix fitting code SAMMY after a semi-empirical estimate of the experimental covariance matrices [5]. In order to determine the effect of this new resonance structure the partial new evaluation has been combined after 'transformation' in to ENDF-6 format with the unadjusted JEF2.2 evaluation.

After the calculation of broad group homogeneous cross sections using the ECCO cell code with these three sets of Pu240 cross section data, spatial calculations have been performed with the ERANOS code scheme to determine the critical mass and the Doppler coefficient for the CIRANO Plutonium Vector configurations and the CAPRA PuN core design. A detailed breakdown of the observed differences over the full reactor spectrum has been made using the perturbation and sensitivity modules of the ERANOS code scheme.

CIRANO Plutonium Vector Configurations

The CIRANO experimental programme performed in the MASURCA facility at Cadarache aims to produce the experimental base required to extend the qualification of the ERANOS formulaire to plutonium burning fast reactor cores. The second part of the CIRANO programme consists of a series of substitution configurations with different plutonium isotopic contents and is known as the Plutonium Vector measurements. Three different types of fuel were used with Pu240 contents of 8%, 18% and 35%, which were named respectively CIRANO ZONA2B POA, CIRANO ZONA2B PIT and CIRANO ZONA2B P2K.

The results for the critical mass of the CIRANO Plutonium Vector configurations are given in Table 1. It can be seen that both the use of the newly evaluated fine resonance structure as well as the ERALIB1 library leads to a reduction in the (E-C)/C value for the critical mass. However the generally good prediction of the critical mass made by all three data sets for each of the plutonium vectors would tend to indicate that the modifications made to the Pu240 cross section data do not have a significant influence on the determination of the critical mass for this type of plutonium oxide fuel (enrichment ~ 25%). A breakdown of the effect of the newly evaluated fine resonance structure for the CIRANO ZONA2B P2K configuration is given in Table 2, and shows the main effect coming from a reduction in the capture contribution in the resonance region (groups 13-26), with the reduction in the fission reaction being negligible by comparison.

CAPRA PuN Core Design

During the first phase of the CAPRA project several different options of 'Pu without U' fuel were considered, and as nitride fuel has long been considered the most serious alternative to oxide fuel, the option PuN was chosen. In this study the PuN fuel considered is that obtained after multi-recycling of MOX fuel in PWR reactors, with a consequently high Pu240 content of approximately 40%. Due to the absence of U238, the importance of Pu240 for the Doppler effect, and the influence of the different data sets will be reviewed.

The differences between JEF2.2 and the newly evaluated resonance parameters and the ERALIB1 data library are shown respectively in Tables 3 and 4 for the critical mass of the CAPRA PuN core. As for the CIRANO Plutonium Vector configurations, it is demonstrated that the adjustments made in the ERALIB1 library are consistent with the newly evaluated fine resonance structure. However, the differences are more marked when compared to the

CIRANO configurations due to the increased Pu240 content. In the resonance region the ERALIB1 adjustments do not go as far as the newly evaluated resonance parameters, a situation which could be improved with the inclusion of integral measurements in the ERALIB1 data base that are more sensitive to the resonance region. Table 5 shows that in the unresolved resonance range there is an inconsistency between the JEF2.2 evaluation and the new resolved cross sections, particularly for the capture and fission cross sections. This inconsistency could be resolved et least by a renormalisation of the unresolved resonance range and the continuum in the JEF2.2 evaluation.

The Doppler effect for the CAPRA PuN core together with the breakdown for the capture and fission contributions is shown in Tables 6 and 7. Although Pu240 gives the predominant contribution to the Doppler effect for the CAPRA PuN core, the different data sets result in a relatively small spread of about 7% in the prediction of the Doppler effect. The newly resolved resonance data gives the largest contribution to the Doppler effect in the resonance region.

Conclusions

An important part of the validation and qualification of the ERANOS formulaire is the associated nuclear data and its suitability for new concepts such as plutonium and minor actinide burning cores. Several studies have shown the influence of Pu240 for the critical mass and sodium void reactivity of plutonium burning cores and this paper reviews the studies performed using Pu240 cross section data from the unadjusted JEF2.2 evaluation, the adjusted ERALIB1 data library, as well as a new evaluation based on measurements performed at ORNL, Hanford and Geel on the resonance region. Two situations have been considered with an important quantity of Pu240: the CIRANO Plutonium Vector measurements and the CAPRA PuN core design.

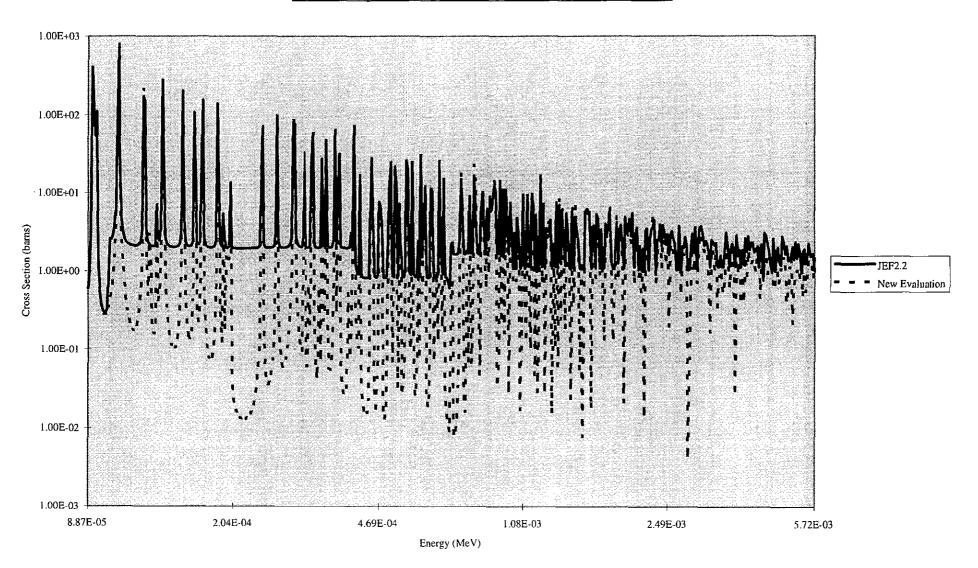
It has been shown that the adjusted cross section data for Pu240 in the ERALIB1 data library is consistent with the differential measurements performed at ORNL, Hanford and Geel. For standard fast reactor cores such as Super-Phénix, as well as the Reference Oxide CAPRA design, as evidenced by the CIRANO experiments, the Pu240 cross section data in the adjusted ERALIB1 data library is considered to be satisfactory. However, for cores such as the CAPRA PuN design where the influence of Pu240 is predominant a complete re-evaluation of Pu240 is required which should take into account the resonance parameters measured at ORNL, Hanford and Geel. A first step in this process could be a renormalisation of the unresolved resonance range or a new calculation of average parameters from sets of the new resolved resonance parameters. In order to fully characterise the CAPRA PuN core design new integral experiments are required. These experiments should provide information in the Pu240 resonance region.

References

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Figure 1: Capture Cross Section for Pu240 in the Resonance Region



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Table 1: Critical Mass of the CIRANO Plutonium Vector Configurations

	ZONA2B POA	ZONA2B PIT	ZONA2B P2K
Standard Calculation			
JEF2.2	1.00625	1.00654	1.00689
ERALIB1	1.00637	1.00685	1.00748
JEF2.2 + New Evaluation	1.00723	1.00763	1.00815
Applied Corrections			
RZ->XYZ	-0.00055	-0.00055	-0.00055
Pu241 Decay	-0.00287	-0.00332	-0.00427
Diffuser	-0.00010	-0.00010	-0.00010
End Caps	+0.00352	+0.00352	+0.00352
Sn	-0.00073	-0.00073	-0.000763
Macrocell	-0.00719	-0.00719	-0.00719
Corrected Calculation	'		
JEF2.2	0.99833	0.99817	0.99757
ERALIB1	0.99845	0.99848	0.99816
JEF2.2 + New Evaluation	0.99931	0.99926	0.99883
Measured Value	0.99882	0.99883	0.99894
(E-C)/C			
JEF2.2	+0.00049	+0.00066	+0.00137
ERALIB1	+0.00037	+0.00035	+0.00078
JEF2.2 + New Evaluation	-0.00049	0.00043_	+0.00011

Table 2 : Perturbation Between the JEF2,2 and JEF2.2+N Evaluation Data Sets for the CIRANO ZONA2B P Configuration (pcm)

GROUP	CAPTURE	FISSION	TRANSPORT	ELASTIC	INELASTIC	N,XN	SUM
1	-1.95	-4.93	0.31	-0.69	-0.86	-2.15	-10.27
2	0.24	-0.63	0.01	-0.13	-0.22	-0.34	-1.07
3	0.05	-0.08	0.06	0.02	-0.04	0.00	0.00
4	0.01	0.12	-0.03	-0.12	-0.06	0.00	-0.08
5	-0.02	0.07	0.01	-0.21	-0.06	0.00	-0.21
6	-0.02	0.08	0.01	-0.09	0.00	0.00	-0.02
7	-0.01	0.07	0.00	10.0-	0.00	0.00	0.05
8	-0.02	0.03	0.00	-0.01	0.00	0.00	0.00
9	0.00	0.02	0.00	0.00	0.00	0.00	0.01
10	-0.01	-0.04	0.00	0.00	0.00	0.00	-0.05
11	0.01	0.12	0.00	0.00	0.00	0.00	0.13
12	0.00	0.00	0.00	0.01	0.00	0.00	0.01
13	20.25	0.06	0.00	0.00	0.00	0.00	20.32
14	12.65	0.02	0.01	0.09	0.00	0.00	12.77
15	2.71	0.01	0.00	0.00	0.00	0.00	2.72
16	0.78	-0.73	0.00	0.04	0.00	0.00	0.08
17	30.49	0.87	0.02	0.25	0.00	0.00	31.63
18	7.97	-2.69	0.00	0.03	0.00	0.00	5.30
19	26.69	-5.69	0.01	0.17	0.00	0.00	21.18
20	14.25	-4.15	-0.03	0.36	0.00	0.00	10.43
21	14.74	-4.93	0.02	0.10	0.00	0.00	9.93
22	9.49	-1.87	0.00	0.36	0.00	0.00	7.97
23	15.54	-2.09	0.07	0.10	0.00	0.00	13.62
24	4.13	-0.82	-0.05	0.16	0.00	0.00	3.42
25	0.14	-0.03	-0.09	-0.01	0.00	0.00	0.00
26	-1.11	0.75	-0.16	0.34	0.00	0.00	-0.18
27	0.10	-0.36	-0.04	-0.12	0.00	0.00	-0.42
28	-1.27	0.39	-0.09	0.00	0.00	0.00	-0.97
29	-0.01	0.00	-0.04	-0.01	0.00	0.00	-0.06
30	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01
31	0.07	-0.02	0.00	-0.01	0.00	0.00	0.05
32	0.00	0.00	0.00	0.00	0.00	0.00	0.01
33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SUM	155.88	-26.45	-0.02	0.63	-1.23	-2.49	126.33

<u>Table 3 : Perturbation Between the JEF2.2 and the JEF2.2+New Evaluation Data Sets for the Critical Mass of the CAPRA PuN Core (pcm)</u>

GROUP	CAPTURE	FISSION	TRANSPORT	INELASTIC	ELASTIC	SUM
1	-0.85604	-0.90675	0.05219	-0.99356	-0.44382	-3.14799
2	0.34757	-0.44217	0.02867	-0.04603	-0.02667	-0.13862
3	0.17058	-0.07463	0.01153	-0.06533	0.11743	0.15958
4	0.07423	-0.02763	0.03071	0.16280	-0.11502	0.12509
5	0.00345	-0.04244	0.01626	-0.06663	-0.22760	-0.31696
6	-0.00458	0.04493	0.01051	-0.04375	0.15979	0.16691
7	0.00863	0.12495	0.01257	-0.01093	0.29478	0.43000
8	-0.02720	0.01242	0.02036	0.00149	0.11296	0.12004
9	0.00125	0.00330	0.00269	0.00112	0.04259	0.05094
10	-0.00605	-0.07541	0.00910	0.00240	0.07820	0.00823
11	0.02874	0.13768	0.00809	0.00222	0.07476	0.25149
12	0.00451	-0.00792	0.00024	0.00072	0.06199	0.05954
13	49.29715	0.00551	-0.00452	-0.00008	-0.02329	49.27478
14	35.79774	-0.05847	0.00392	0.00003	0.00509	35.74830
15	9.12946	-0.00509	0.00016	-0.00001	-0.01675	9.10777
16	3.36371	-2.35714	-0.00606	0.00007	0.03454	1.03512
17	151.08410	-0.23574	-0.07758	0.00000	0.13367	150.90450
18	52.05963	-15.08064	-0.00178	0.00000	0.02317	37.00038
19	142.09880	-27.65641	-0.01141	0.00000	0.46958	114.90060
20	90.88609	-23.28587	0.01487	0.00000	1.86063	69.47572
21	130.99430	-37.36908	-0.00326	0.00000	-0.63074	92.99119
22	112.07190	-19.47043	0.00015	0.00000	2.80016	95.40176
23	176.00510	-26.00158	0.01776	0.00000	-0.70448	149.31680
24	49.89116	-8.74938	-0.01735	0.00000	1.78325	42.90768
25	3.37439	-1.70038	-0.03015	0.00000	-0.27495	1.36891
26	-4.14323	-1.35970	-0.03367	0.00000	-0.01242	-5.54902
27	2.86285	-0.58776	-0.01931	0.00000	-0.00474	2.25104
28	-3.00929	0.45194	-0.01980	0.00000	-0.01088	-2.58803
29	-0.02136	0.01076	-0.00804	0.00000	-0.00020	-0.01883
30	-0.00164	0.00413	-0.00541	0.00000	-0.00062	-0.00354
31	0.19620	-0.07967	0.00010	0.00000	-0.03245	0.08418
32	0.00905	-0.00302	0.00002	0.00000	0.00000	0.00605
33	0.00059	0.00003	0.00000	0.00000	0.00000	0.00062
PART >0	-8.06939	-165.57730	-0.23833	-1.22631	-2.52463	-177.63600
PART <0	1009.76100	0.79566	0.23988	0.17086	8.05259	1019.02000
SUM	1001.69200	-164.78170	0.00155	-1.05545	5.52795	841.38420

<u>Table 4 : Perturbation Between the JEF2.2 and the ERALIB1 Data Sets for the Critical Mass of the CAPRA PuN Core (pcm)</u>

GROUP	CAPTURE	FISSION	TRANSPORT	INELASTIC	ELASTIC	SUM
1	0.78156	0.25879	0.11143	-0.55148	-0.01895	0.58134
2	5.39370	1.77199	0.44184	-0.87944	0.01900	6.74710
3	15.38549	6.54689	-4.55007	-0.87736	-0.26075	16.24421
4	19.87455	5.30392	-14.09029	7.03907	1.07223	19.19948
5	21.63834	-20.77853	-23.48648	2.55892	7.77615	-12.29161
6	38.29227	-27.77633	-82.15721	10.41514	34.68299	-26.54315
7	73.03874	0.59774	-72.66132	6.31720	56.51765	63.81001
8	76.22910	10.87454	-42.05428	-0.37186	26.23922	70.91672
9	74.04985	8.12792	-33.84623	-0.30147	20.73340	68.76346
10	87.31282	5.97343	-40.65079	-0.19031	23.79096	76.23611
11	70.96003	0.22338	-22.29594	-0.12054	15.06655	63.83349
12	58.88906	-4.93796	-10.74253	0.02622	9.32800	52.56279
13	53.65801	-9.19181	-4.45582	0.04464	2.41626	42.47128
14	45.10160	-10.56276	-4.02945	-0.00633	1.98016	32.48323
15	47.03526	-14.07436	-2.27363	-0.00018	0.93873	31.62582
16	18.26986	-11.74458	-0.59907	-0.00028	-0.03156	5.89437
17	9.43401	-14.88476	-0.46190	0.00000	0.03542	-5.87723
18	3.68720	-9.06267	-0.11810	0.00000	-0.06549	-5.55906
19	4.85760	-30.71810	-0.41400	0.00000	-0.12566	-26.40015
20	-66.85541	-17.01716	-0.26789	0.00000	-1.69384	-85.83430
21	-5.87554	-4.11945	-0.21652	0.00000	0.71150	-9.50001
22	14.29831	-10.37455	-0.04995	0.00000	-0.54361	3.33020
23	8.87076	-19.04952	0.25829	0.00000	0.05326	-9.86722
24	5.17468	-5.35583	0.19372	0.00000	0.01768	0.03026
25	1.81646	-2.98085	0.13540	0.00000	0.12477	-0.90423
26	-0.17285	-1.50041	0.24800	0.00000	-0.02469	-1.44995
27	-0.63709	-1.04732	0.12029	0.00000	0.02445	-1.53966
28	0.76798	0.05645	0.07959	0.00000	-0.00362	0.90041
29	-0.01204	-0.03689	0.03976	0.00000	0.04474	0.03558
30	-0.06911	-0.09562	0.02281	0.00000	-0.08353	-0.22545
31	0.06537	-0.00384	0.00083	0.00000	-0.00770	0.05466
32	0.04918	0.00239	0.00154	0.00000	-0.00246	0.05065
33	0.00446	0.00041	0.00068	0.00000	0.00000	0.00556
PART > 0	-73.62202	-215.31330	-359.42150	-3.29923	-2.86187	-654.51790
PART < 0	754.93620	39.73786	1.65419	26.40119	201.57310	1024.30300
SUM	681.31420	-175.57540	-357.76730	23.10196	198.71130	369.78470

<u>Table 5 : Consistency Between the JEF2.2 Unresolved Cross Sections and the Newly Resolved Cross Sections for the Energy Range 4 KeV - 5.7 KeV</u>

	JEF2.2	New Evaluation	Difference (%)
Total Cross Section	18.46	17.68	-4.4
Scattering Cross Section	16.68	16.5	-1.0
Fission Cross Section	0.089	0.097	+8.55
Capture Cross Section	1.69	1.06	-60.0

Table 6: Doppler Effect for the CAPRA PuN Core: 700°C -> 300°C (pcm)

	JEF2.2	JEF2.2 + New Evaluation	ERALIB1
Pu239	-2.9	-6.9	-5.4
Pu240	-216.3	-228.6	-207.1
Pu241	+4.7	+4.6	+4.6
Pu242	-29.3	-31.4	-28.3
Fe	-81.2	-83.3	-85.9
Total	-325.0	-345.6	-322.1

<u>Table 7: Breakdown of the Doppler Effect for the CAPRA PuN Core (pcm)</u>

		F2.2		ew Evaluation	ERALI	
GROUP	CAPTURE	FISSION	CAPTURE	FISSION	CAPTURE	FISSION
1	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	-0.01	0.00	-0.02	0.00	-0.02
7	0.00	-0.04	0.00	-0.05	0.00	-0.04
8	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00
12	-0.01	0.00	-0.01	0.00	-0.01	0.00
13	-0.25	0.03	-0.25	0.03	-0.24	0.02
14	-0.51	0.07	-0.52	0.06	-0.48	0.06
15	-0.95	0.11	-0.95	0.11	-0.89	0.10
16	-1.15	0.08	-1.20	0.04	-1.09	0.07
17	-1.51	0.08	-1.75	0.22	-1.44	0.06
18	-1.83	0.44	-2.23	0.39	-1.75	0.37
19	-12.45	2.03	-15.29	1.81	-11.99	1.71
20	-22.67	3.70	-32.85	3.95	-21.77	3.17
21	-27.28	-4.92	-24.53	0.66	-26.24	-4.26
22	-21.55	0.33	-16.59	0.17	-20.29	0.30
23	-52.07	0.52	-55.55	0.39	-49.34	0.47
24	-34.94	0.38	-38.10	0.04	-33.50	0.35
25	-18.13	0.15	-20.02	0.04	-17.45	0.13
26	-14.36	0.13	-15.65	0.01	-13.94	0.12
27	-5.81	0.06	-6.29	0.00	-5.67	0.05
28	-3.70	0.03	-4.42	0.04	-3.52	0.03
29	0.00	0.00	0.00	0.00	0.00	0.00
30	0.00	0.00	0.00	0.00	0.00	0.00
31	-0.45	0.00	-0.45	0.00	-0.43	0.00
32	0.00	0.00	0.00	0.00	0.00	0.00
33	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL	-219.62	3.13	-236.66	7.91	-210.04	2.69