INTERFERENCE EFFECTS BETWEEN RESONANCE ABSORBERS

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ABSTRACT

Multigroup shielded cross sections have been generated using continuous energy Monte Carlo calculations in homogeneous mixtures of resonance absorbers and hydrogen. In contrast to the conventional methodology of solving the slowing down equation in homogeneous mixtures of single heavy absorber and a light moderator, three component mixtures have been examined to treat the resonance interference (and overlap) effects between two resonant nuclides. Since U-238 is the most important resonance absorber in reactor fuels, homogeneous mixtures of U-238 and other absorbers such as U-235, Pu-239, and Pu-240 have been considered in the present study. The background cross section provided by U-238 is representative of typical fuel compositions. The concentration of the second component was varied to derive a set of background cross sections for this (the second) absorber. Extensive tables of resonance group cross sections were generated using MCNP 4B (1) as a function of temperature and background cross sections for U-235, Pu-239, and Pu-240. Significant differences between the cross-sections from the conventional NJOY (2) procedure and the multi component MCNP calculations were noticed in the energy groups where there were resonances of both the absorbers. These differences can not be accounted for accurately through the standard techniques of including the resonance interference effects. Finally, the impact of the modified resonance group cross sections on the reactivity predictions of some benchmarks has been examined. It is found that the agreement between MCNP and deterministic calculations improves significantly using the newly generated tables of resonance integrals.

1. INTRODUCTION

Self shielded cross sections for the multigroup libraries are generally derived from the flux computed in infinite homogeneous mixtures of a single heavy absorber and a light moderator. Solution of the integral slowing down equation provides the point-wise flux in these mixtures

which is then used as the weighting function to evaluate the group cross sections. Extensive tabulations of resonance integrals as a function of temperature and background cross sections are generated in this way for the resonance absorbers of interest in the physics design of reactors(2).

However, in practice, reactor fuel rarely contains only one single isotope. U-235 and U-238 are always present together in varying concentrations. Also isotopes of plutonium build up with fuel irradiation. Resonances in one isotope will interfere with those in the others. For example, the low energy resonances of U-238 (at 6.67, 20.87, 36.68, 66.03 eV) cause strong dips in the flux distribution in and around the resonance energy. If the other isotopes have resonances in the vicinity of these, the flux distribution will be significantly different than that in the single component mixture. U-235, Pu-239, and Pu-240 have very important resonances in the proximity of the above U-238 resonances affecting not only their own cross sections but the cross sections of other absorbers as well.

Williams(3) has provided an excellent overview of the physical effects of resonance interference (and overlap) phenomena in a mixture of resonance absorbers. He introduced a factor to account for the effect that the resonances of one material have on the weighting function used in averaging the cross sections of another resonant nuclide. The computation of this "additional" factor to be used in conjunction with the previously generated resonance tabulations was based on the Wide Resonance approximation. His calculations indicated that the incorporation of this factor improved the performance of the standard self shielding method significantly. Group cross sections could change by as much as 40 % as a result of the interference between the resonances of mixed absorbers.

In practice, the interaction effects between resonance absorbers are accounted through an iterative procedure. This involves the modification of the background cross section of a given absorber by the sum of the absorption cross sections of all the other absorbers in the mixture at the second (and higher) iterations. Normally, only one iteration is assumed to adequately represent the interference effects (4).

In spite of some weak links, this procedure works satisfactorily for the low enrichment lattices and also when the plutonium isotopic contents are small. But with high enrichments used (and also highly burnt fuels) in modern PWRs, the interaction effects cannot be accounted for in a satisfactory manner through this simplistic but desirable approach. This became very apparent during the qualification of our ENDF/B-VI (5) based multigroup library (6) against MCNP for Doppler Defect benchmarks proposed by Mosteller (7). The results are in an unpublished report by the author.

We noticed that the differences between the deterministic calculations and ENDF/B-VI based 70-group library and the continuous energy Monte Carlo calculations had an increasing trend with enrichment. The multigroup library had included a reduction of 3.4 % (8) in the total resonance integral of U-238, while the MCNP continuous energy cross sections had no such adjustment made for U-238 resonance captures. Increasing the number of iterations to treat the interference effects did not help to improve the situations. Mark Williams (3) and T. Takeda (9) provided a clue to have a second look at the standard methodology.

NJOY(1) has an option to use the flux calculated in the mixture of one resonance isotope as the weighting function for averaging the cross sections of another resonance material. For example, the flux from the mixture of U-238 and hydrogen may be supplied as the weighting function in the mixture with U-235 or Pu-239 as the resonant isotope.This will definitely help to correct for the interaction effects at the library stage itself. However, this option has the implicit assumption of making the Narrow Resonance approximation for the second (U-235 or Pu-239) absorber. This approximation is not valid especially for the low energy resonances of the heavy absorbers. On the other hand, Williams correction factors were based on the Wide Resonance approximation.

Using the special option of NJOY, we observed significant differences in the infinitely dilute resonance integrals of the second absorber – as much as 10 %. Obviously, this was not acceptable.

2. CALCULATION OF RESONANCE INTEGRALS

In view of the limitations of the two methods described above, we decided to perform continuous energy Monte Carlo calculations using MCNP to account for the additional complication of the flux shape caused by the resonances of U-238 in the proximity of resonances of U-235 (or Pu-239). Once again, following the conventional wisdom, only infinite homogeneous mixtures were considered.

The background cross section for U-238 in the mixture was representative of typical UO2 fuel rods. The concentration of the second absorber in the mixture was varied to realize the sets of background cross sections needed for tabulating the shielded resonance integrals.

Continuous energy cross sections were first generated using NJOY at several temperatures for U-235, U-238, Pu-239, Pu-240, and H-1. It must be emphasized here that no adjustment was made in the continuous energy cross sections of U-238. Nearly, two million neutron histories were covered in each calculation to reduce the relative errors in reaction rate tallies to an acceptable level. Absorption and nu-fission rates were combined with the corresponding fluxes to derive the group resonance integrals as required by our multigroup library structure.

The resonance group cross sections for U-238 did not show any significant effect coming from the interaction of resonances of U-235, while U-235 cross section did exhibit significant changes in groups where the flux dips caused by U-238 resonances were appreciable. The group boundaries of the 17 groups in the resonance range are described in Table I. Percentage changes in the group resonance integrals of U-235 in each of the 17 groups of the resonance range, are given in Table II. These are listed at typical back ground cross sections. As can be seen, the total infinitely dilute integrals are not affected very much, which is contrary to what was observed using the NJOY option of using the flux from mixture as the weighting function in the mixture of another absorber.

For Pu-239 and Pu-240, the resonance group cross sections show much larger changes than those in U-235. These results are shown in Tables III and IV. The impact on the resonance integrals are in conformity with the observations and (the results) of previous publications (3,9).

Table I. Group Boundaries (eV) in the Resonance Range

Gp	Upper	Lower
1.	9118.0	5530.0
2.	5530.0	3519.1
3.	3519.1	2239.45
4.	2239.45	1425.1
5.	1425.1	906.898
6.	906.898	367.262
7.	367.262	148.728
8.	148.728	75.5014
9.	75.5014	48.052
10.	48.052	27.700
11.	27.700	15.968
12.	15.968	9.877
13.	9.877	4.000
14.	4.000	3.300
15.	3.300	2.850
16.	2.850	2.500
17.	2.500	2.100

Table II. Resonance Interference Effect on U-235 Absorption and Nu-fission Integrals As a Function of Background Cross-section

	Absorption					Nu fission				
Gp	655	1048	1361	2419	Inf	655	1048	1361	2419	Inf
1	-.05	-.11	-.01	.02	.01	-.11	-.05	.00	.02	.01
2	.00	-.07	.02	.07	.07	-.07	.00	.02	.07	.07
3	-.01	-.06	.04	.07	.02	-.07	-.01	.03	.07	.02
4	.10	.20	.11	.01	.06	.08	-.05	-.06	-.18	-.19
5	.70	.84	.73	.73	.72	1.23	1.06	1.16	1.06	1.10
6	.55	.50	.40	.42	.32	.65	.72	.54	.53	.47
7	.12	.21	.02	-.01	-.22	.92	.78	.69	.65	.49
8	.75	.78	.45	.39	.14	.40	.38	.14	.10	-.03
9	2.49	2.41	2.60	2.90	2.49	2.79	2.81	2.83	3.13	2.85
10	3.89	4.52	3.65	3.71	2.64	3.93	3.29	3.10	3.18	2.13
11	-5.20	-4.59	-5.58	-6.28	-7.95	-.46	-.87	-1.21	-1.81	-3.31
12	.91	.98	.98	.59	-.28	.78	.51	.61	.28	-.34
13	1.20	1.86	1.22	.15	-.45	7.97	7.77	7.96	7.32	7.23
14	1.03	.67	.69	.43	.60	.59	1.05	.75	.44	.65
15	-.10	.09	-.08	.08	.03	.09	-.10	-.09	.07	.03
16	-.05	.08	-.03	-.06	-.11	.11	-.11	.01	-.05	-.10

17	.10	.07	.23	.11	.02	.02	.02	.09	.05	.02
Sum	.49	.78	.38	.05	-.67	2.31	2.17	2.14	1.97	1.58

Table III. Resonance Interference Effect on Pu-239 Absorption and Nu-fission Integrals As a Function of Background Cross-section

	Absorption					Nu fission				
Gp	655	1048	1361	2419	Inf	655	1048	1361	2419	Inf
1	.23	.18	.12	.06	.00	.24	.20	.16	.09	.00
2	.52	.33	.25	.15	-.02	.48	.32	.24	.16	.02
3	1.19	.86	.74	.65	.37	1.04	.76	.70	.57	.30
4	.05	-.12	-.11	-.39	-.50	-.60	-.80	-.86	-1.13	-1.13
5	-3.03	-3.03	-3.41	-3.31	-3.72	-3.47	-3.53	-3.79	-3.66	-3.95
6	2.85	2.85	3.12	2.91	2.91	2.36	2.34	2.55	2.41	2.62
7	2.87	2.48	1.86	1.62	.68	1.89	1.45	1.30	1.01	.17
8	2.77	3.17	2.23	2.10	1.45	2.58	2.94	2.38	2.30	1.98
9	-1.94	-2.77	-2.98	-4.43	-6.08	-2.98	-3.95	-4.20	-5.64	-7.57
10	12.25	11.55	10.21	10.04	7.21	10.55	9.67	9.38	8.47	7.01
11	10.10	9.41	9.36	8.59	7.19	10.15	9.41	9.38	8.56	7.07
12	.68	.68	.75	1.12	-.05	.30	.34	.47	.93	.05
13	10.55	10.93	11.37	10.76	9.90	8.69	9.30	9.81	9.40	8.89
14	-.10	-.08	-.09	-.10	-.07	-.10	-.08	-.09	-.10	-.07
15	-.02	-.04	-.03	-.03	-.01	-.02	-.03	-.03	-.03	-.01
16	-.03	-.05	-.04	-.05	-.05	-.03	-.05	-.04	-.05	-.05
17	-.05	-.09	-.09	-.10	-.08	-.05	-.08	-.09	-.10	-.08
Sum	3.69	3.57	3.41	3.16	2.12	2.57	2.45	2.47	2.25	1.45

Table IV. Resonance Interference Effect on Pu-240 Absorption and Nu-fission Integrals As a Function of Background Cross-section

	Absorption					Nu fission				
Gp	3000	5000	10000	40000	Inf	3000	5000	10000	40000	Inf
1	.36	.25	.22	.13	.13	.28	.22	.13	.12	.07
2	.79	.83	.90	1.23	.93	-.06	-.04	.22	1.18	.81
3	1.39	1.25	.93	.69	.92	2.85	5.15	2.94	3.20	1.32
4	.82	1.43	1.45	.77	1.27	3.82	4.57	4.84	2.73	5.32
5	-.66	-1.73	-2.33	-2.50	-2.85	2.30	2.86	1.86	2.47	1.20
6	2.92	2.15	2.36	2.04	2.02	-.62	-2.15	-.51	-.32	-1.89
7	7.89	8.05	7.79	7.20	7.34	5.96	6.15	5.63	5.08	5.40
8	3.65	1.69	-.24	-1.02	-.59	5.17	3.35	2.83	3.09	2.28
9	-15.80	-20.25	-30.02	-32.11	-35.54	-2.92	-3.70	-10.16	-10.32	-11.85
10	10.19	6.16	2.80	1.74	1.07	8.00	2.94	-.90	-2.37	-2.90
11	-38.56	-45.94	-52.65	-54.97	-54.10	-38.74	-46.15	-52.87	-55.20	-54.32
12	-.06	-.06	-.07	-.05	-.05	-.03	.00	-.09	-.05	-.10
13	1.70	1.80	1.76	1.68	1.74	.65	.68	.67	.64	.67
14	.09	.14	.10	.11	.02	.05	.08	.06	.06	.02

15	.07	.00	-.11	.00	.04	.05	.00	-.08	.00	.02
16	-.03	-.03	-.03	.03	-.03	-.03	-.02	-.02	.02	-.02
17	.13	.01	.13	.02	.16	.11	.01	.11	.02	.13
Sum	-1.84	-4.94	-8.44	-9.56	-10.13	-4.20	-5.68	-7.23	-7.84	-8.34

3. RESULTS AND CONCLUSIONS

The new resonance integral tabulations have been inserted in a prototype version of the 70-group library. At the same time, calculation of the shielded cross sections was also modified so as not to double count the interference effects. The new version showed considerable improvement in the comparison of deterministic predictions to MCNP results. Most of the differences observed earlier were reduced significantly. This is true, in particular, for the Doppler Coefficient benchmarks. Deltak/k (with reference to our earlier unpublished results) are listed in Table V. It might be added here that we have extended the range of enrichments vis a vis the original Mosteller paper. The reactivity effect is a strong function of U-235 enrichment - it may be as large as 0.3 %.

Table V : Reactivity Impact of Interference Between U-235 and U-238 as a Function of U-235 Enrichment

	Enr	dk/k (%)	
	w/o	HZP	HFP
1	0.71	.09	.09
2	1.60	.14	.14
3	2.40	.17	.18
4	3.10	.20	.21
5	3.90	.23	.24
6	4.20	.24	.25
7	4.50	.25	.26
8	4.80	.25	.27

In order to evaluate the impact of changes in the Pu-239 and Pu-240 cross sections as a result of interference of U-238 resonances, we repeated the calculations for some MOX critical experiments (6) with varying plutonium isotopic compositions. Comparison of these results is shown in Table VI. As has been indicated by other researchers (3,9), the overall reactivity impact of variations in the Pu-239 and Pu-240 resonance cross sections is very small. The maximum effect noticed for these criticals is about 0.06 %. Small impact on the reactivity of the MOX criticals is perhaps due to the fact that the most important resonance of the plutonium isotopes are in the thermal range while the current study evaluated the impact from the epithermal range.

Table VI : Impact on Reactivity of Resonance Interference Between U-238, Pu-239, and Pu-240 - MOX Critical Experiments

a) ESADA Uniform Lattice Critical Experiments With 2.0 w/o PuO2 in Natural UO2

S.N.	Lattice Pitch(In)	Boron PPM	dk/k (%) U-235	Pu-239	Pu-240
1	0.69	0	.04	-.03	.02
2	0.75	0	.03	-.02	.01
3	0.9758	0	.02	-.01	.01
4	1.0607	0	.01	-.01	.00
5	1.380	0	.01	.00	.00
6	0.69	261	.04	-.02	.02
7	0.9758	261	.02	-.01	.01
8	0.69	526	.04	-.02	.02
9	0.9758	526	.02	.00	.01
10	0.9758(*)	0	.02	.00	.01
11	1.0607(*)	0	.01	.00	.01

b) SAXTON Uniform Lattice Critical Experiments with 6.6 w/o PuO2 in 5.74 w/o UO2

S.N.	Lattice Pitch(In)	Boron PPM	dk/k (%) U-235	Pu-239	Pu-240
1	0.52	0	.03	-.06	.026
2	0.56	0	.02	-.05	.024
3	0.56	327	.02	-.04	.024
4	0.735	0	.01	-.03	.011
5	0.792	0	.01	-.03	.018
6	1.04	0	.01	-.01	.009

(*) Pu-240 Isotopic Content is 24 %. All others have 8 % Pu-240 Content

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