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Sensitivity of reactor multiplication factor to positions of cross-section resonances

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Abstract. Neutron–nuclear interaction cross-section is sensitive to neutron kinetic energy and most nuclei exhibit resonance behaviour at specific energies within the resonance energy range, spanning from a fraction of an electron volt to several tens or hundreds of kilo electron volts. The energy positions of these resonances correspond to the excitation energy levels of the compound nucleus that are formed as intermediate states during the interaction. Though these positions, thanks to sophistication in science and technology, are known reasonably precisely for the materials of reactor interest, deviations or spread in this data among different evaluations cannot be ruled out. In this work, the effect of such a spread in the resonance positions of the reactor materials on the multiplication factor of an infinite reactor, is obtained. The study shows that the effect on a thermal reactor is more pronounced than on a fast reactor.

Keywords. Nuclear data; cross-sections; resonances; fast reactor; thermal reactor; reactivity.

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1. Introduction

The physics design of a reactor core, and study of its behaviour while it is in a steady state of operation or otherwise, needs the neutron–nuclear interaction cross-sections as precisely as possible. The cross-sections of relevant reactions are the essential input quantities to solve the neutronics equations that predict the state of a reactor. The cross-section for any specific reaction depends sensitively on the kinetic energy of the neutron and on the nuclide it collides with. The typical variation of cross-section σ with neutron kinetic energy E is drastically fluctuating in the so-called 'resonance energy range' whose extent is different for different nuclides. Such a resonance structure is predominantly seen for elastic scattering, radiative capture, fission and hence total cross-sections. Certain other reactions like inelastic scattering can also have resonances. The (n, α) reaction of ^{59}Ni shows a resonance structure.

Resonance structure in cross-sections are due to the excitation energy levels of the compound nucleus (CN), an energetically excited system formed as an intermediate state with the target nucleus having absorbed the incoming neutron, during a reaction process [1,2]. A CN is formed at an energy level E^* if the kinetic energy E_0 of the neutron plus the binding energy of the neutron in the CN equals E^*. E_0 is identified as a resonance position. Though well-known, the following is included for a completeness and to give a clue on the difficulties in resonance data specifications.

The evaluated nuclear data files/libraries are major sources of nuclear data for reactor physics and other purposes. 'Evaluation' of nuclear data considers a large mass of available measured data, which are sparse in some respects and excessive in some other respects, prunes them carefully, selects the best data, and fills the gaps through data obtained based on nuclear reaction models, and through suitable interpolations. Internationally well-known evaluated data files, such as ENDF/B-VII (American) [3], JENDL-4 (Japanese) [4] and JEFF-3 (European) [5] are some of the recently released state-of-the-art databases, distributed by international data centres like the International Atomic Energy Agency (IAEA) [6], Vienna, Austria, in computer-readable standardized formats [7]. An evaluated database is expected to consist of complete and consistent data, for any nuclide listed therein. A neutron cross-section data file covers an energy range from 10^{-5} eV to 20 MeV generally, and a larger range in certain cases.

Owing to the multiplicity of the measured and predicted databases considered, the associated experimental and modelling uncertainties, added to the subjective interpretations of the evaluating teams, it is natural to see a spread in the evaluated quantity. However, the spread has been found to become smaller with advancing science and technology. The resonance data measurements and data reduction are specifically complicated due to rapid fluctuation in the cross-sections over small energy intervals. The parametrization of the data to fit them into suitable mathematical formalisms involves quantum mechanical treatment. Complication also arises due to the resolution and Doppler broadening. Further, as the energy resolution becomes worse and the density of levels increases with excitation energy, identification of individual resonances is rendered difficult at higher energies in the resonance range. Recognition of an 'unresolved resonance range' (URR) within the resonance energy range, at higher energies than the 'resolved resonance range' (RRR), is due to this problem [8]. Thus, the resonance range is a challenge to the evaluation, and very efficient codes like SAMMY [9] deal with this challenge laudably.

The boundaries of the resonance range, and those of the URR and RRR are obviously not uniquely definable, and could vary between evaluations for a given nuclide. The number of resonances in the RRR, and the specification of the resonance parameters could also vary between two independent evaluations. Thus, apart from the experimental uncertainties, there could exist a spread in the data specifications.

A small shift in the resonance position with no change in the other parameters will make the point cross-sections differ by several orders of magnitude due to the rapid variation typical of any resonance behaviour. However, this is not likely to affect the predicted integral parameters badly, because the average cross-section over a region of energies will not be affected significantly. It should further be remembered that the RRR of the fuel is below the region where the flux peaks in a fast reactor (FR), and well above that in a thermal reactor (TR). Therefore, in this work, wherein the effect of slightly shifting (perturbing) the resonance positions in the RRR on the predicted multiplication factor (k) of a reactor is being assessed, the deviations expected are small. The effect depends on the flux spectrum of the system, the RRR, in addition to its material composition.

'Shift' in this context only indicates a perturbation in the position of a resonance, not affecting the other independent parameters of the function describing a resonance. Essentially, the aim of this paper is not to alarm the user, as if a large spread is observed among the present evaluations. Spread between truly independent evaluations is natural and the scientific curiosity to see its effect is the motivation for this work.

In this work, a uniform infinite mixture of fuel and structural nuclides with composition typical of an FR core, and a uniform infinite natural uranium core of a TR are considered. The resonance positions in each of the materials in the mixture are shifted, one material at a time, from -2% to $+2\%$ of their initial positions. The cross-section reconstruction from the resonance parameters is done using the IAEA PREPRO [10]/RECENT code and averaging is done using indigenous codes. k_∞ is calculated as the ratio of neutron production to absorption in the composite medium using macroscopic one-group average cross-sections.

Resonance self-shielding effect was found to be below 1% due to the resonance shifting on the one-group capture cross-sections of ^{238}U at a target temperature of 300 K, for a near-realistic dilution cross-section of 100 barns in a FR spectrum (see results shown in §4.3.1). Self-shielding effects are not considered further for the present study.

2. Data preparation

2.1 *Representation of resonance cross-sections*

In an evaluated nuclear data file (ENDF), as per the latest standard format viz. ENDF-6 [7], the cross-sections in the RRR are given through resonance parameters fitted to a recognized formalism, in a portion of data called 'file2' (i.e. MF = 2). The URR gives only average data corresponding to clusters of resonances. In the present work, URR for any material is taken as it is in the database. Besides, the cross-section σ vs. the neutron kinetic energy E, for every reaction, is generally given as a table on a suitable energy grid, with an apt interpolation scheme, in a portion of data called 'file3' (MF = 3). In file3, the value given at E in the resonance energy region is not the cross-section value but the correction (say $\pm\delta\sigma$) to be added to the σ obtained at that E based on the resonance parameter data. These corrections are known as 'background corrections' or 'floor corrections'. The background corrections in the RRR are ignored in this work. This should not significantly affect the difference between the values calculated before and after the shifting, as the background is neglected in both. It is also shown herein (see §4.2) that the effect of excluding the background on k_∞ is indeed very small, for the cases studied here.

2.2 *Resonance data processing*

The LINEAR and the RECENT programs of the latest IAEA preprocessing code system, viz. PREPRO (2015)

[10] are used. The LINEAR and RECENT programs recast the resonance parameter data given in file2 and the table of σ vs. E given in file3 into a new table wherein linear interpolation is applicable, within a desired tolerance, between any pair of successive tabulated energies. The fineness of the energy grid is increased to achieve this. As expected, the data-size grows manifold after these processing steps. At the end of this step, linearly interpolable cross-sections are available in tabular forms for every reaction.

2.3 *Multigroup and one-group cross-section averages*

Neutronics core calculation method [8] generally employs 'multigroup' average cross-sections, in which the whole energy range considered (usually the upper limit is less than 20 MeV) is split into some number, NG, of groups (intervals of energy) and average cross-sections obtained within each group as in eq. (1).

$$\sigma_{xg} = \int_g \sigma_x(E)\phi(E)\,\mathrm{d}E \Big/ \int_g \phi(E)\,\mathrm{d}E. \tag{1}$$

In eq. (1), g is the group index (g = 1, 2, 3,..., NG) and ϕ is the neutron flux in the reactor. The flux-weighting ensures conservation of total rate of the reaction x in the group. The total group flux ϕ_g is given by the denominator of eq. (1). In the absence of an *a-priori* knowledge of $\phi\,(E)$, some approximate slowly varying function $S(E)$ (say, $1/E$) is used for the above multigroup averaging. Through a neutronics (diffusion or transport) calculation using σ_{xg} as the input, the multigroup fluxes ϕ_g are calculated, appropriate to the reactor system considered.

With σ_{xg} and ϕ_g known, the one-group cross-section $\langle\sigma\rangle_x$, representing the average over the entire energy range, may be calculated as

$$\langle\sigma\rangle_x = \sum_g \sigma_{xg}\,\phi_g \Big/ \sum_g \phi_g, \tag{2}$$

where the summation is over all the NG groups.

3. The methodology

3.1 *The multiplication factor*

With the requisite nuclear data prepared as above, for all the nuclides of a reactor core, the multiplication factor k may be calculated as the ratio of the rate of production and the rate of loss of neutrons. In this work, the intention is not to obtain the realistic multiplication factor of a reactor core, but, as said earlier, is to calculate the difference in k due to a difference in the resonance energy positions of a particular nuclide. Accordingly, the reactor core is considered to consist of a uniform mixture of constituent nuclides and to extend to infinity. The infinite size avoids loss of neutrons through leakage; hence the neutron loss is only through absorption. In the one-group treatment, the neutron production is only through fission. Hence, the multiplication factor is given by

$$k_\infty = \sum_i a_i \langle\nu\sigma\rangle_{fi} \Big/ \sum_i a_i(\langle\sigma\rangle_{fi} + \langle\sigma\rangle_{ci}). \tag{3}$$

In eq. (3), a_i represents the number density of nuclide the i in the mixture. The quantities $\langle\nu\sigma\rangle_{fi}$, $\langle\sigma\rangle_{fi}$ and $\langle\sigma\rangle_{ci}$, respectively represent average production, fission and capture cross-sections of the nuclide i, ν symbolizes the number of neutrons produced per fission. The summations are over all the nuclides in the mixture including fuel and non-fuel nuclides.

3.2 *Procedure followed*

All the component nuclides of the core mixture are selected from the ENDF and a small file is created, wherein the file3 (background) corrections are made zero. This remains the source nuclear data file for the entire calculations. All the resonance positions in the RRR of one material are shifted by a desired percentage compared to the original positions, with all the other nuclides unchanged. The modified data are pre-processed using LINEAR and RECENT and multigroup and hence one-group cross-sections are obtained using known multigroup fluxes. With known number densities of the mixture components, k_∞ is calculated. The procedure is repeated for -2%, $+2\%$, -1% and $+1\%$ shifts, and the results are compared with that for unchanged data (i.e. 0% shift). Many of the non-fuel materials (like Fe, Cr, Ni) have several isotopes each. In such cases, the same percentage shift is given for each of the isotope in an element, and the elemental cross-sections are prepared using isotopic abundance weighting. One material (one isotope for fuel nuclides but one element for non-fuel nuclides) at a time is thus modified.

4. Present calculations, results and discussion

4.1 *Group limits, flux spectra and atom densities*

Table 1 gives the energy limits and the multigroup flux spectra used for 25 group structures for the FR and 69 group structures for the TR studies. The FR fluxes are the results of an earlier neutronics calculation for a commercial level fast breeder reactor (FBR) core. Table 2 gives the atomic number densities (in units of

Table 1. Energy group limits and normalized fluxes in the fast and the thermal reactors.

Fast reactor			Thermal reactor								
g	E_g (eV)[a]	ϕ_g	g	E_g (eV)	ϕ_g	g	E_g (eV)	ϕ_g	g	E_g (eV)	ϕ_g
1	1.45E+7	1.161E−2	1	1.00E+7	4.602E−5	27	9.88E+0	3.068E−5	53	2.50E−1	1.064E−3
2	3.68E+6	2.846E−2	2	6.07E+6	1.749E−4	28	4.00E+0	6.529E−6	54	2.20E−1	4.967E−3
3	2.23E+6	4.474E−2	3	3.68E+6	3.058E−4	29	3.30E+0	8.092E−6	55	1.80E−1	1.918E−2
4	1.36E+6	5.353E−2	4	2.23E+6	3.250E−4	30	2.60E+0	7.249E−6	56	1.40E−1	6.916E−2
5	8.22E+5	9.976E−2	5	1.35E+6	2.524E−4	31	2.10E+0	1.142E−5	57	1.00E−1	8.095E−2
6	4.99E+5	8.610E−2	6	8.21E+5	1.609E−4	32	1.50E+0	4.857E−6	58	8.00E−2	8.184E−2
7	3.02E+5	1.205E−1	7	5.00E+5	8.288E−5	33	1.30E+0	4.161E−6	59	6.70E−2	7.424E−2
8	1.83E+5	1.065E−1	8	3.25E+5	5.899E−5	34	1.15E+0	8.064E−7	60	5.80E−2	7.972E−2
9	1.11E+5	9.795E−2	9	1.83E+5	2.461E−5	35	1.12E+0	7.951E−7	61	5.00E−2	9.310E−2
10	6.75E+4	8.252E−2	10	1.11E+5	1.696E−5	36	1.10E+0	8.141E−7	62	4.20E−2	9.166E−2
11	4.09E+4	7.739E−2	11	6.73E+4	1.697E−5	37	1.07E+0	8.342E−7	63	3.50E−2	7.007E−2
12	2.48E+4	6.823E−2	12	4.09E+4	1.697E−5	38	1.05E+0	8.219E−7	64	3.00E−2	7.221E−2
13	1.51E+4	3.767E−2	13	2.48E+4	1.697E−5	39	1.02E+0	8.082E−7	65	2.50E−2	7.194E−2
14	9.13E+3	2.967E−2	14	1.50E+4	1.696E−5	40	9.96E−1	8.279E−7	66	2.00E−2	6.811E−2
15	5.54E+3	1.209E−2	15	9.12E+3	1.697E−5	41	9.72E−1	7.771E−7	67	1.50E−2	5.917E−2
16	3.36E+3	1.108E−2	16	5.53E+3	1.534E−5	42	9.50E−1	1.460E−6	68	1.00E−2	4.307E−2
17	2.04E+3	1.768E−2	17	3.52E+3	1.534E−5	43	9.10E−1	2.315E−6	69	5.00E−3	1.710E−2
18	1.24E+3	9.184E−3	18	2.24E+3	1.534E−5	44	8.50E−1	2.917E−6	70	1.00E−5	
19	7.50E+2	3.420E−3	19	1.43E+3	1.534E−5	45	7.80E−1	7.520E−6			
20	4.55E+2	1.381E−3	20	9.07E+2	3.068E−5	46	6.25E−1	7.574E−6			
21	2.76E+2	4.722E−4	21	3.67E+2	3.068E−5	47	5.00E−1	7.574E−6			
22	1.01E+2	8.516E−5	22	1.49E+2	2.301E−5	48	4.00E−1	1.225E−5			
23	2.26E+1	4.442E−6	23	7.55E+1	1.534E−5	49	3.50E−1	2.924E−5			
24	3.06E+0	8.763E−8	24	4.81E+1	1.870E−5	50	3.20E−1	4.714E−5			
25	4.14E−1	1.81E−10	25	2.77E+1	1.870E−5	51	3.00E−1	9.718E−5			
26	1.00E−5		26	1.60E+1	1.631E−5	52	2.80E−1	3.671E−4			

[a]Upper energy limit.

Table 2. Number densities of the reactor components.

		Atom densities (10^{24}/cm^3)	
Nuclide/element	MAT[a]	Fast reactor	Thermal reactor
Na	1100	8.9907E−03	
Cr	2400	2.9966E−03	
Mn	2500	4.0518e−04	
Fe	2600	1.3169E−02	
Ni	2800	2.8440E−03	
^{235}U	9228	1.3500E−05	3.41725E−4
^{238}U	9237	5.4001E−03	4.78650E−2
^{239}Pu	9437	9.6466E−04	
^{240}Pu	9440	3.4497E−04	
^{241}Pu	9443	7.3762E−05	
^{242}Pu	9446	1.8931E−05	

[a]Material identifier in ENDF-6 convention.

10^{24} atoms per cm^3) for the same FBR core composition. The TR fuel is considered to be made up of only natural uranium whose atom densities are also given. The TR flux spectra given are the group integrals of fission spectrum, $1/E$ spectrum and Maxwellian spectrum, respectively, in the high, intermediate and thermal energy regions.

4.2 *Differences in resonance data evaluations*

Table 3 compares the salient details of RRR data between ENDF/B-VII.1 [3] and JENDL-4.0 [4] evaluations, abbreviated herein for ease of reference as E7 and J4, respectively. Only the nuclides relevant to this study are included. The present day evaluations mostly specify

Table 3. Resolved resonance region data in ENDF/B-VII.1 (E7) and JENDL-4 (J4).

Nuclide	MAT	Evaluation	Formalism	E_{low} (eV)	E_{high} (eV)	No. of l values	No. of resonances
^{23}Na	1125	E7	MLBW	6.00E+2	5.00E+5	3	23
		J4	MLBW	1.00E−5	3.50E+5	3	20
^{50}Cr	2425	E7	RM	1.00E−5	7.83E+5	3	393
		J4	RM	1.00E−5	6.00E+5	3	114
^{52}Cr	2431	E7	RM	1.00E−5	1.43E+6	3	392
		J4	RM	1.00E−5	1.43E+6	3	392
^{53}Cr	2434	E7	RM	1.00E−5	5.64E+5	2	350
		J4	RM	1.00E−5	5.64E+5	2	350
^{54}Cr	2437	E7	RM	1.00E−5	8.34E+5	3	118
		J4	RM	1.00E−5	7.50E+5	2	110
^{55}Mn	2525	E7	RM	1.00E−5	1.25E+5	2	187
		J4	RM	1.00E−5	1.25E+5	2	187
^{54}Fe	2625	E7	RM	1.00E−5	7.00E+5	3	380
		J4	RM	1.00E−5	7.00E+5	3	380
^{56}Fe	2631	E7	RM	1.00E−5	8.50E+5	4	311
		J4	RM	1.00E−5	8.50E+5	3	313
^{57}Fe	2634	E7	RM	1.00E−5	2.00E+5	3	75
		J4	RM	1.00E−5	2.00E+5	2	50
^{58}Fe	2637	E7	RM	1.00E−5	4.00E+5	3	68
		J4	RM	1.00E−5	3.50E+5	2	68
^{58}Ni	2825	E7	RM	1.00E−5	8.12E+5	3	493
		J4	RM	1.00E−5	8.12E+5	3	482
^{60}Ni	2831	E7	RM	1.00E−5	8.00E+5	3	480
		J4	MLBW	1.00E−5	4.56E+5	3	278
^{61}Ni	2834	E7	MLBW	1.00E−5	5.70E+4	2	57
		J4	MLBW	1.00E−5	5.70E+4	2	57
^{62}Ni	2837	E7	MLBW	1.00E−5	6.00E+5	2	79
		J4	MLBW	1.00E−5	5.57E+5	2	82
^{64}Ni	2843	E7	MLBW	1.00E−5	5.53E+5	2	63
		J4	MLBW	1.00E−5	5.53E+5	2	63
^{235}U	9228	E7	RM	1.00E−5	2.25E+3	1	3193
		J4	RM	1.00E−5	5.00E+2	1	3193
^{238}U	9237	E7	RM	1.00E−5	2.00E+4	2	3343
		J4	RM	1.00E−5	2.00E+4	2	3343
^{239}Pu	9437	E7	RM	1.00E−5	1.00E+3	1	405
				1.00E+3	2.00E+3	1	441
				2.00E+3	2.50E+3	1	224
		J4	RM	1.00E−5	2.50E+3	1	1046
^{240}Pu	9440	E7	MLBW	1.00E−5	5.70E+3	1	268
		J4	RM	1.00E−5	2.70E+3	1	434
^{241}Pu	9443	E7	RM	1.00E−5	3.00E+2	1	244
		J4	RM	1.00E−5	3.00E+2	1	244
^{242}Pu	9446	E7	MLBW	1.00E−5	9.23E+2	2	65
		J4	MLBW	1.00E−5	1.00E+3	1	101

the lower limit (E_{Low}) of RRR as 10^{-5} eV. However, E7 gives it as 600 eV for Na-23. We can see varying specifications for the upper limits (E_{high}), the l-values (neutron angular momentum) and the number of resonances. Further, the formalisms specified are also different in some cases. It could be seen that the RRR is split into three subregions for ^{239}Pu in E7, but has only one region in J4. Some nuclides, say ^{238}U, have identical data indicating common data source for both the evaluations. ^{235}U shows identical number of resonances in E7 and J4, but the resonance ranges given are very different. In figure 1 are given the multigroup normalized flux spectra for the

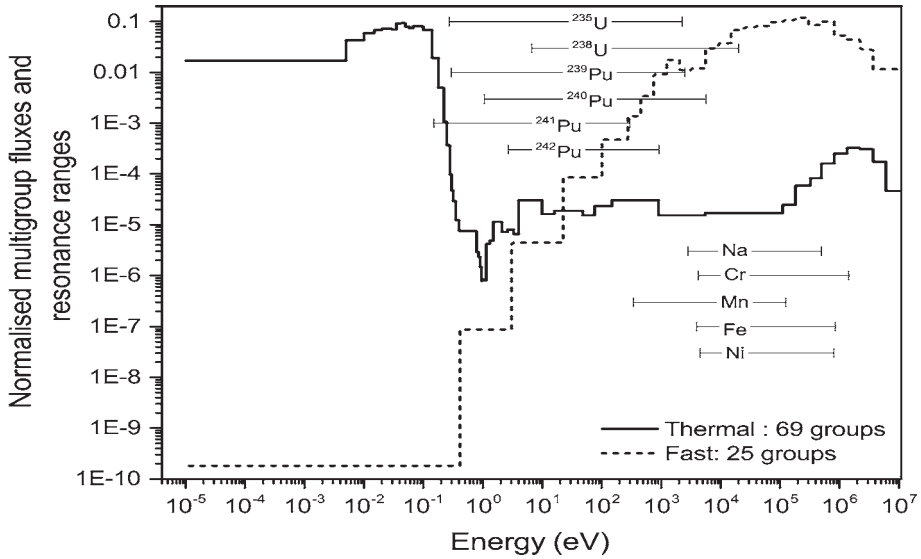

Figure 1. Multigroup fluxes and the resonance ranges.

Table 4. Deviation in k_∞ when RRR parameters of E7 are replaced with J4.

Nuclide whose RRR parameters are replaced		Deviation in k_∞ from E7 (%)	
Nuclide	MAT	Background neglected E7 $k_\infty = 1.47443$	Background included E7 $k_\infty = 1.47449$
Cr	2400	0.0071	0.0071
Mn	2525	0.0000	0.0000
Fe	2600	−0.0005	−0.0003
Ni	2800	−0.1539	−0.1530
^{235}U	9228	−0.0268	−0.0267
^{238}U	9237	0.0000	0.0000
^{239}Pu	9437	−5.0178	−4.9990
^{240}Pu	9440	1.2125	1.2083
^{241}Pu	9443	−1.2467	−1.2423
^{242}Pu	9446	0.0973	0.0970

TR and the FR. The resonance range for each material is indicated by a horizontal line drawn from the energy position of the first resonance up to E_{high}.

With respect to the resonance positions for the nuclides considered in this work, E7 and J4 do not differ much. However, due to the other differences mentioned above, the effect of replacing E7 RRR parameters with the J4 parameters is found to be considerable. Multigroup and hence one-group cross-sections are prepared from E7, as per procedures discussed earlier, for an FR nuclide composition. Then one-group cross-sections are prepared with E7 RRR parameters replaced with J4 parameters, for each of the material, one at a time. Background corrections are ignored in all the cases. Table 4 compares k_∞ computed with E7 and J4 parameters. There is no deviation for ^{238}U because the E7 and J4 parameters are identical. Large deviation of 5% (5000 pcm) is seen for ^{239}Pu. ^{240}Pu and ^{241}Pu also show large deviations of about 1.2% (1200 pcm), though their fractions in the mixture are relatively much smaller. The motivation for the present work stems from such deviations. It can be seen from table 4 that the effect of ignoring the background corrections (see §2.1) is not very significant on k_∞.

4.3 *Observations*

It must be remembered that larger the original energy position of a resonance, the larger also is its actual shift, for any percentage shift. The FR is a ^{239}Pu/^{238}U oxide fueled FBR of about 3000 l core capacity and 1200 MWt

Table 5. Relative deviations in k_∞ due to resonance shifts in a fast reactor core mixture (reference k_∞ value: 1.47443).

Material whose resonance positions are shifted		Deviations ($\Delta k/k_\infty$) for various shifts in resonance positions (pcm)					
Material	MAT	−1%	+1%	RMS	−2%	+2%	RMS
^{238}U	9237	−211.91	261.89	238.21	−402.17	538.91	475.48
^{235}U	9228	0.44	−0.58	0.51	0.74	−0.82	0.78
^{239}Pu	9437	−5.10	−18.68	13.69	11.17	−29.06	22.01
^{240}Pu	9440	−12.98	16.74	14.98	−25.18	31.41	28.47
^{241}Pu	9443	0.11	−0.31	0.23	0.60	−0.27	0.47
^{242}Pu	9446	−0.57	−0.27	0.45	−0.92	−0.26	0.68
Cr	2400	−8.33	8.27	8.30	−16.42	16.02	16.22
Mn	2525	−5.66	5.08	5.38	−11.34	10.49	10.92
Fe	2600	−43.03	42.55	42.79	−86.28	80.24	83.31
Ni	2800	−15.76	14.76	15.27	−31.60	30.13	30.87
Na	1100	−8.59	7.93	8.27	−16.84	16.06	16.45
^{238}U + ^{239}Pu	9237+9437	−216.87	243.35	230.49	−390.46	510.55	454.49
All		−317.7	338.14	**328.08**	−575.68	696.00	**638.68**
Effective $\Delta k/k_\infty$ in pcm* =				**243.70**			**485.72**

RMS: Root-mean-square of the values in the preceding two columns.
*Root of sum of squared RMS values of individual materials.
Bold values indicate effective or aggregate values

power, whose core fluxes are used herein. The natural uranium thermal reactor could be taken as a PHWR.

4.3.1 *Results for FR.* Table 5 gives the results of the present calculations for a FR. k_∞ calculated with the unmodified resonance parameter data is 1.47443 and the relative deviations ($\Delta k/k_\infty$) for the modified cases are compared with this value. Resonance shifts of ±1% and ±2% are considered, in the resonance positions of the individual nuclides and k_∞ computed for the mixture for each modification in the data. The following are observed from table 5:

- Resonance shifting in ^{238}U has the maximum deviation, due to its being the most dominant nuclide in the fuel, and to its RRR spreading to energy regions of greater fluxes than ^{239}Pu. The deviations are near 250 pcm (1 pcm = 10^{-5} of reference k_∞) and near 500 pcm for ±1% and ±2% shifts, respectively.
- ^{239}Pu shows moderate deviations below 30 pcm. Unlike ^{238}U whose effect is only due to capture, ^{239}Pu effect is due to fission and capture. This is the reason for the negative deviations for −1% and +1% shifts.
- ^{240}Pu, though occupies much less fraction in the fuel, shows deviation comparable to that of ^{239}Pu due to its larger RRR.
- Structural materials and sodium also show significant deviations, with iron exceeding 40 pcm for ±1% shift, and 80 pcm for ±2% shift.
- The averages, in a root-mean-square (RMS) sense, are given for individual nuclides, for the ±1% and ±2% cases. The effective or potential deviation due to an assumed percentage spread in the resonance positions in all the nuclides is obtained as the square root of the sum of the squares of these individual RMS values. It is seen that the effective deviation for the spread within ±1% is about 243 pcm and that for the ±2% spread is about 486 pcm. It may be noted that 243 pcm is approximately 0.7$ reactivity of a typical FBR (1$ of a typical FBR would be around 350 pcm).
- However, when the resonance shifting is done in all the materials of the mixture, the calculated RMS values for $\Delta k/k_\infty$ are 328 and 640 pcm, for the ±1% and ±2% shifts, respectively, becoming more significant with respect to 1$.
- It is interesting to note, in most cases, that the effect of shifting nearly doubles when the shift percentage is doubled.
- As mentioned in the Introduction, the net effect expected is small. The reason is that the RRR for the nuclides, excepting the structural ones, are at low energies where the neutron flux in a FR is low. The one-group treatment considered spans the entire energy range and dilutes the changes in the RRR. With this taken into consideration, a relative deviation of over 200 pcm in k_∞, for the RRR resonance shifts within ±1% seems considerable. The resonance shift of ±2% is, probably, an unrealistic spread

Table 6. Relative deviations in k_∞ due to resonance shifts in a thermal reactor core mixture (reference k_∞ value: 1.327667).

Nuclide whose resonance positions are shifted		Deviations ($\Delta k/k_\infty$) for various shifts in resonance positions (pcm)					
Nuclide	MAT	−1%	+1%	RMS	−2%	+2%	RMS
^{235}U	9228	−19.00	22.00	21.00	−40.00	42.00	41.00
^{238}U	9237	−776.00	787.00	781.00	−1599.00	1564.00	1581.00
^{235}U and ^{238}U	9228+9237	−794.00	810.00	**802.00**	−1636.00	1609.00	**1622.00**
Effective $\Delta k/k_\infty$ in pcm* =				**782.00**			**1582.00**

RMS: Root-mean-square of the values in the preceding two columns.
*Root of sum of squared RMS values of individual nuclides.
Bold values indicate effective or aggregate values

in the resonance energy specifications, but it helps to observe that the deviation in k grows approximately as the percentage shift.

It is well-known that resonance self-shielding is the most important for ^{238}U capture. It was independently found that the self-shielded one-group capture cross-section of ^{238}U at 300 K for a near-realistic dilution of 100 barns, in a FR, is 0.28143 b. For the resonance shifts of −2%, −1%, +1% and +2%, the value deviates by 0.725%, 0.384%, −0.320% and −0.792%, respectively. Since the deviation is less than 1% due to shifting, the self-shielding effects are not considered in this study.

4.3.2 *Results for TR.* Table 6 gives similar results for a TR. Natural uranium with heavy water moderator makes a mixture of a TR. However, the absorption in the moderator being negligible, the TR is assumed to be made up of natural uranium for the present calculations. Thus, k_∞ of natural uranium is considered with flux spectrum and cross-sections corresponding to a TR. The relative deviations in k_∞ are given in pcm. The reference k_∞ for the unmodified data is 1.327667.

The observations from table 6 are:

- The deviations are about 800 pcm and 1600 pcm for the ±1% and ±2% cases, respectively, and are almost due to ^{238}U. As the flux varies as $1/E$ in the resonance region, the dominant ^{238}U capture resonances see lower fluxes when shifted to the right and higher fluxes when shifted to the left, leading to the observed deviations.
- Here again, the doubling effects are seen as for the FR.
- The net reactivity observed in the FR as well as in the TR are almost contributed by ^{238}U, and it is seen that the effect of spread in the resonance positions on a TR is about three times the effect in FR.
- The reactivity associated with a ±1% spread in the resonance positions of ^{238}U is more than 1$ of a typical natural uranium TR (1$ of a natural uranium fueled reactor would be less than 600 pcm).

4.3.3 *Resonance integrals.* The effect of spread in the resonance positions on the capture and fission resonance integrals (RI) were also calculated using

$$\mathrm{RI} = \int \sigma(E)(1/E)\mathrm{d}E, \tag{4}$$

between a lower limit of 10^{-5} eV and an upper limit covering the URR (if any). The RI values differ well within 5%, and the results are not shown here.

5. Conclusions

The effect of possible spread in the resonance positions of reactor core materials on the multiplication factor of a reactor was studied, with assumed shifts of ±1% and ±2% in the resonance energies. An infinite homogeneous nuclide mixture with composition typical of a fast breeder reactor, and an infinite natural uranium mixture of a thermal reactor were considered. Using one-group neutron cross-sections, infinite multiplication factor and relative deviations in it, due to the resonance shifting in individual nuclides and in all of them, were calculated. As expected, ^{238}U shows the highest deviation, followed by iron. For the ±1% shifts in all the nuclides in the fast reactor case, the net relative deviation is about 330 pcm, which is close to 1$ reactivity therein. The value doubles for ±2% shift. In the case of thermal reactor, the deviations are 800 pcm, i.e. greater than 1$ reactivity for ±1% shift and 1600 pcm for ±2% shift.

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