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Evaluation of Statistical Resonance Parameters for ^{232}Th in 4 to 41 keV Energy Region

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ABSTRACT

In this note, the author presents an exhaustive compilation of mean resonance parameters for ^{232}Th isotope reported by different experimental groups, evaluators and users. A set of mean resonance parameters is obtained for ^{232}Th for use in reactor calculations by adjusting the p wave strength function as a function of energy region for a broad group structure corresponding to the already evaluated total and partial cross sections recommended in the ENDF/B-IV library in 4 to 41keV energy region. The difficulties associated with the evaluation of mean resonance parameters for given evaluated cross sections in the unresolved resonance region are highlighted. A brief comparison of the American ENDF/B procedure and the German KEDAK procedure for the processing of the unresolved resonance data is also given. A possibility exists to explain part of the discrepancies between the calculated and the experimentally determined integral parameters to be due to the non-uniqueness of the mean resonance parameters in the unresolved resonance region for the main fissile and fertile nuclides. It appears more satisfying to evaluate the mean resonance data (and hence the self shielded cross sections) for a given multigroup structure used in reactor calculations unlike the ENDF/B convention. We further recommend that the thick sample transmission and self-indication measurements be performed for ^{232}Th in order to determine experimentally the self shielded cross sections in the unresolved resonance region and to support the above mentioned evaluation of mean resonance parameters.

EVALUTION OF STATISTICAL RESONANCE PARAMETERS FOR ^{232}Th IN 4 TO 41 keV ENERGY REGION

S. Ganesan

1. INTRODUCTION

The neutron induced reaction rates in the unresolved resonance energy region are of fundamental importance in the calculation of important integral parameters such as K_{eff}, breeding ratio and reactivity coefficients (Doppler and sodium void reactivity effects) of large fast reactor systems. For thorium fuelled fast reactors, the evaluation of statistical resonance parameters for ^{232}Th is thus of great importance. The difficulties experienced in the representation of cross sections in the unresolved resonance region in general, for the main fissile and fertile isotopes have been reviewed by many workers in the past.[1-7] The evaluated nuclear data files[4,5] describe the cross sections in the unresolved resonance region in terms of the statistical resonance parameters, i.e. the mean values of these resonance parameters and the distribution functions obeyed by these parameters. This means that, in the unresolved resonance region, the cross sections are not unique but are defined by probability distributions[1,2] for the various cross sections of thorium. The unresolved resonance region for ^{232}Th starts from 4 keV onwards[8]. While recommendations[7] have been made to abandon the statistical approach and made direct use of the data obtained in the high resolution cross section measurements, the reactor designers may still have to rely on the statistical approach[1,2] till acceptable high resolution cross section measurements are made available for the neutron induced reactions in ^{232}Th. Thus in this note based on the statistical approach, we perform the evaluation of the mean resonance parameters in 4 to 41 keV energy region for ^{232}Th corresponding to the already evaluated cross sections recommended in the ENDF/B-IV file[8], using the ADDJA code[6] developed at

Reactor Research Centre, Kalpakkam for such evaluations. The reason for our truncating the higher energy limit at 41 keV is merely that beyond this energy region the Doppler broadening/ self-shielding effects are not significant for all practical purposes of calculations of temperature and composition dependent self-shielded cross sections which are used in fast reactor calculations. It should further be borne in mind that this Note concentrates only on those aspects associated with the evaluation of mean resonance parameters and not on the evaluation of partial and total cross sections themselves in 4 to 41 keV energy region. As such the already evaluated cross sections available in the ENDF/B-IV file are chosen as those cross sections which are to be reproduced well by the mean resonance data set to be evaluated in this paper.

2. Status of Mean Resonance Parameters for ^{232}Th

The mean resonance parameters given in the evaluated nuclear data files [4,5] for describing the cross sections in the unresolved resonance energy region obey the usual statistical formalism[1,2]. The following nomenclature is used throughout in this note.

$\langle \sigma_{nx} \rangle (\bar{E})$: Cross section for the process x at the average energy; x can be c or f or n; n-neutron scattering; f-fission; c-capture.

σ_p : Background potential scattering cross section

λ : $\lambda/2\pi$ where λ is the wave length of the neutron.

I, J : Spins of the target and compound nuclides respectively.

g_J : Statistical spin factor $= \dfrac{2J + 1}{2\ (2I + 1)}$.

ℓ : Angular momentum of the incident neutron.

$\langle D \rangle^{(\ell,J)}$: Mean level spacing for the sequence defined by (ℓ,j).

$\overline{\Gamma}_x^{(\ell,J)}$: Mean partial reaction width for the process x for the energy $\overline{E}$ for the sequence (ℓ,j).

$\Gamma^{(\ell,J)}$: Total reaction width = $\sum_x \overline{\Gamma}_x^{(\ell,J)}(\overline{E})$ for the sequence (ℓ,j).

$\nu_x^{(\ell,J)}$: Degrees of freedom for the Porter-Thomas distribution for the process x.

$\langle \phi \rangle_{(\ell,J)}$: These brackets denote averaging of the function within the bracket over appropriate Porter-Thomas distribution functions obeyed by the partial reaction widths $\overline{\Gamma}_x^{(\ell,J)}$ and $\langle D \rangle^{(\ell,J)}$.

S_ℓ : Strength function for the ℓth partial wave; ℓ = 0 corresponds to the s waves and ℓ = 1 to the p waves.

While the various mean resonance parameters are derived from the statistics of the resolved resonances, some parameter, p wave strength function for instance, is adjusted to reproduce the evaluated cross sections in the unresolved resonance region. Even when a particular reaction formalism has been employed, considerable discrepancies exist in the various mean resonance parameters reported for various fertile and fissile nuclei by various authors.[6] The mean resonance parameters for ^{232}Th as compiled by us from different sources are given in Table I to amply illustrate this point. We find from the values given in Table I, that some mean resonance parameters are discrepant by several tens of percent. The reasons for the large discrepancies among these even when a particular reaction formalism (the statistical formalism of

TABLE I

A COMPILATION OF MEAN RESONANCE PARAMETER FOR ^{232}Th

Quantity	$\ell = 0$		$\ell = 1$	
	$J = \frac{1}{2}$		$J = 3/2, \frac{1}{2}$	
$\langle D \rangle^{(\ell,J)}$ (eV)	17.00	(44,45)	8.5	(44)
	12.95	(8)	6.475	(8)
	16.70	(9)	8.35	(9)
	24.30	(10)	11.80	(10)
	20.10	(12)	10.0	(12)
$\langle D \rangle^{(0,\frac{1}{2})} = \langle D \rangle^{(1,\frac{1}{2})}$	19.00	(13)	9.5	(13)
	22.7	(40)	11.4	(40)
$S_\ell \times (10^4)$	0.73	(8)	1.2	(8)
	0.84 ± 0.08	(9)	0.9	(9)
	0.695 ± 0.088	(10)	1.43 ± 0.17	(10)
	0.888	(44,45)	0.9 ± 0.4	(11)
	0.85 ± 0.88	(11)	1.0	(12)
	0.632	(12)	2.06	(13)
	0.70		1.9	(15)
	0.365 ± 0.024	(39)	2.0	(16)
	0.793	(40)	0.55	(17)
			1.078 ± 0.057	(39)
			1.718	(40)** (S_1, J=3/2 =1.711 (S_1, J=1/2 =1.718
$\overline{\Gamma_\gamma}^{(\ell,J)}$	0.0213	(44)		
	0.0259	(8)		
	0.0219 ± 0.009	(9)		
	0.0212 + 0.0028	(10)		
	0.03	(12)		
	0.0245	(14)		
	0.0198	(39)		

(** In Ref. 40, S_1 depends on J)

Lane & Lynn[2]) is employed for a given nuclide are the following :

1. Discrepancy exists in the recommended capture or fission or total cross sections themselves or the values of alpha (= σ_c / σ_f) to which the adjustment of mean resonance parameters is made.

2. The method of evaluation of mean resonance parameter itself can be different along with the discrepancies which exist in other parameters used in the evaluation process.

3. The mean resonance parameters for the unresolved resonance region are derived from the statistics of the resolved resonance parameters. In some reaction formalisms, (multilevel formalism, for example) the resonance parameters themselves are not unique, even for a given cross section behaviour. In some cases the statistics of the resolved resonance region may be inadequate.

3. CALCULATIONS OF INFINITE DILUTION CROSS SECTIONS

As seen in Table I, while some evaluators[15,17] provide only a particular mean resonance parameter such as radiative width or s and p wave strength functions, we also note that complete sets of evaluated mean resonance parameters are available from some sources[8,9,12] Defining that one set of mean resonance parameter consists of $\langle D \rangle^{(\ell,J)}$ $\overline{\Gamma}_x^{(\ell,J)}$ and S_ℓ for all values of ℓ and j, and the radius of the nucleus, we find that many consistent sets of mean resonance parameters can be formed by making combinations (based on individual judgement which may sometimes be even simply canonical) of values given in Table I. However, we realise that all such sets will not lead to the same infinite dilution cross sections recommended by, say a particular evaluator.

The ENDF/B-IV data for $\langle \sigma_t \rangle (\bar{E})$ and $\langle \sigma_{n\gamma} \rangle (\bar{E})$ for ^{232}Th are given in Ref. 8. We give following linear relation for the

behaviour of the mean capture cross section for ^{232}Th in 4 keV to 40 keV energy region.

$$\langle \sigma_{n\gamma} \rangle (\bar{E}) = 1.15 - \frac{0.75}{37} (\bar{E} - 3) \quad (1)$$

where $\bar{E}$ is in keV. This equation is easily obtained by reading the $\langle \sigma_{n\gamma} \rangle (\bar{E})$ values at 3 and 40 keV energies from Ref. 8 and assuming the linear relation between $\langle \sigma_{n\gamma} \rangle$ and $\bar{E}$ to hold between these energy points as recommended by Witkopf[8].

In the statistical formalism[1,2], the cross sections are calculated using the following expression:

$$\langle \sigma_{nx} \rangle (\bar{E}) = 2\pi^2 \lambda^2 \sum_{(\ell,J)} g_J \frac{\left\langle \frac{\Gamma_n^{(\ell,J)}(\bar{E}) \Gamma_x^{(\ell,J)}(\bar{E})}{\Gamma^{(\ell,J)}(\bar{E})} \right\rangle_{(\ell,J)}}{\langle D \rangle^{(\ell,J)}} \quad (2)$$

$$\sigma_t (\bar{E}) = \sigma_p + \sum_x \langle \sigma_{nx} \rangle (\bar{E}) \quad (3)$$

The expectation value $\langle \sigma_{nx} \rangle (\bar{E})$ is conveniently assumed to represent the value of these quantities for an energy width ΔE for which the mid point is $\bar{E}$ and for the energy region for which the mean resonance parameters S_ℓ, $\langle D \rangle^{(\ell,J)}$, $\Gamma_x^{(\ell,J)}$ are given.

In Table II, we have formed six (complete) sets of mean resonance parameters which are chosen from the values compiled in Table I. While each set of mean resonance parameter is taken from a single source as far as possible we fill the gap, wherever the data is lacking, by drawing the appropriate parameter from the first set. It is customary to accept a set of mean resonance parameters if they produce the infinite dilution cross sections which are in 'good' agreement with the recommended cross sections. How 'good' this agreement should be, and actually is, again depends on the evaluator. We calculated the values of

TABLE II

A FEW SETS OF MEAN RESONANCE PARAMETERS

Set No.	Description of mean resonance parameter
1.	Ref. (8)
2.	Ref. (9)
3.	Ref. (10) with radiation width from Ref. (8)
4.	Ref. (10) for S_1 and Ref. (8) for other parameters
5.	Ref. (12)
6.	Ref. (13) with radiation width from Ref. (8)

$\langle \sigma_{n\gamma} \rangle (\bar{E})$ and $\langle \sigma_{E} \rangle (\bar{E})$ by using each of the six sets of mean resonance parameters in Eq.(2) which is based on the statistical formalism. We found that the sets 1,3 to 6 reproduce approximately the ENDF/B-IV values even though the agreement is not uniform in the entire energy region for each of these sets.

4. ON THE RECOMMENDATION OF A SET OF MEAN RESONANCE PARAMETERS

While a set of cross sections given by an evaluator may be accepted based on its ability to reproduce certain integral parameters of the reactor system under study, it has been observed in particular that the Doppler and sodium reactivity coefficients depend sensitively on the selected set of mean resonance parameters. We recall here[6] that there can exist different sets of consistent mean resonance parameters leading to the same values of infinite dilution cross sections but giving rise not only to different values of self shielding factors but also to different values of temperature derivative of the self shielding factor. In other words, for such sets of mean resonance parameters, while the infinite dilution cross sections are the same, the relative changes in scattering, capture and total reaction processes, as the temperature and composition are varied do not remain to be the same. Thus the fate of the neutrons entering the energy group or the change in the ratio of the increase in neutron population from one generation to another is different for a given temperature change for the different sets of mean resonance parameters. This introduces an uncertainty[6] in the calculation of Doppler coefficient of reactivity in large fast reactor systems, the amount of uncertainty being dependent on the choice of the set of mean resonance parameters used in the calculations.

In general, the determination of the p wave strength functions is considerably more difficult than that of s wave strength function because the identification of the small p wave resonance is difficult in the

resolved resonance region. Further, the assignment of ℓ value for an observed small resonance is uncertain. For instance, the latest measurement of ^{232}Th resonance parameters as published in 1972 by Rahn et. al.,[9] includes a significant number of levels as compared to the measurements carried out earlier[18] in 1964 by the same experimental group. While, as pointed out by Goldsmith[15], a theoretical calculation of the p wave strength function is desirable, we obtain the p wave strength function, for each energy group by fitting it to the evaluated partial and total cross sections. This process of getting a set of mean resonance parameters has an advantage. It removes the uncertainty which creeps in when, while doing sensitivity studies, a reactor designer simply chooses a set of mean resonance parameters which gives 'good' (but not exact) agreement with the given evaluated values of the recommended partial and total cross sections for the various energy groups in the unresolved resonance region. In other words, when the effect of uncertainty in the evaluated cross sections is being tested with respect to a particular integral parameter, care is taken to see that the mean resonance parameters used in the calculations, at least reproduce exactly the evaluated values of the total and the partial cross sections in each energy group, so as to make the sensitivity studies more credible. However, the basic uncertainty in the very choice[6] of the mean resonance parameter and the inherent statistical error[19,20] in the statistical approach do remain unaffected by the procedure.

5. EFFECT OF UNCERTAINTIES IN OTHER MEAN RESONANCE PARAMETERS USED ON THE EVALUATION OF p WAVE STRENGTH FUNCTION

It is clear that the p wave strength function so evaluated has its associated uncertainty because of uncertainties in other mean resonance parameters S_ℓ, $\langle D \rangle^{(\ell,J)}$, $\bar{\Gamma}_x^{(\ell,J)}$ and the nuclear radius. A series of parametric studies performed using ADDJA code[6]

to understand these effects are made as follows :

The uncertainty in the nuclear radius affects the evaluation of the p wave strength function at energies where the $\ell = 1$ sequences are important. The ENDF/B format convention uses, for the nuclear radius an expression of the form $R = (a\ A^{1/3} + 0.8) \times 10^{-13}$ cm where 'a' is a constant. The value of $R = 0.965\ (\text{barn})^{\frac{1}{2}}$ used in this report corresponds to a value of the constant 'a' = 1.44. The value of 'a' varies from 1.2 to 1.5 in the literature. However, for our discussion, we would like to state that an uncertainty of $\sim$3% in nuclear radius parameter introduces an uncertainty of $\sim$ 6% in the evaluated p wave strength function. We also investigated the impact on the adjusted p wave strength function corresponding to two values of s wave strength function whose value is varied from 0.65×10^{-4} to 0.85×10^{-4}.

At lower energies, the evaluation of p wave strength function is considerably affected (to about 40%) by the assumed values of the s wave strength function. Physically this is expected as only at higher energies the contributions to the cross sections coming from the p waves are larger. We calculated the adjusted values of S_1 corresponding to two values of s wave level spacing (10.95 eV and 14.95 eV). It is seen that the (15%) uncertainty in s wave level spacing introduces in the adjusted p wave strength function large uncertainties ($\sim$ 50%) at lower energies and less ($\sim$ 15%) at higher energies. This is physically expected since the contributions of the p waves to the cross sections are less at lower energies. For a lower value of s wave level spacing ($\langle D \rangle^{(0,J)}$ = 10.95 eV) the adjusted values of S_1 are smaller. This is understood from the fact that when the s wave level spacing is smaller, the contribution of s wave to the cross section is larger. Similarly only at higher energies the impact of the uncertainty in $\langle D \rangle^{(1,\frac{3}{2})}$ on the evaluation of S_1 is felt. In this section, we have essentially demonstrated the nonuniqueness of the set of mean resonance parameters corresponding to a given mean cross section. The non-uniqueness of p wave strength function has arisen because of nonunique-

ness of other mean resonance parameters used in the evaluation process.

6. AN ADJUSTED SET OF MEAN RESONANCE PARAMETERS FOR ^{232}Th.

A set of adjusted mean resonance parameters which reproduce the values $\langle \sigma_{n\gamma} \rangle (\bar{E})$ and $\langle \sigma_t \rangle (\bar{E})$ given in ENDF/B-IV [8] is presented in Table III. The $\flat$ wave strength function is the mean resonance parameter obtained by adjustment to fit the values of $\langle \sigma_{n\gamma} \rangle (\bar{E})$ and $\langle \sigma_t \rangle (\bar{E})$. The adjustment was performed using ADDJA code [6]. The other mean resonance parameters used in this evaluation process have been drawn from set No. 1 (see Table II), the reason for which is simply that we wanted to stick to the recommended values given already in ENDF/B-IV file. Both the values of $\langle \sigma_t \rangle$ and $\langle \sigma_{n\gamma} \rangle$ calculated using the mean resonance data set recommended in Table III are in excellent agreement (within about 1.5%) with those recommended in ENDF/IV in the energy region 4 to 41 keV. It should be noted that the measured total cross sections for ^{232}Th in the unresolved resonance region reported by the experimenters have an experimental uncertainty about 4%. The experimental uncertainty in $\langle \sigma_{n\gamma} \rangle$ which is difficult to measure directly is not less than $\pm$ 10% in the unresolved resonance region. An idea of the uncertainties associated with the cross section measurements for ^{232}Th can be found in the work of Meadows et al. [41] for the energy range 49 keV to 20 MeV. (Note further that the report by Meadows et al. [41] does not deal with the evaluation of statistical resonance parameters which are dealt with in the present paper).

We note in Table III that the adjusted $\flat$ wave strength function rises by nearly a factor of 3 in 20keV and drops back by some factor in the next 20 keV. While such a behaviour of the $\flat$ wave strength function is also an accepted practice in ENDF/B circles it is satisfying to observe that this variation in the adjusted $\flat$ wave strength function is within the

TABLE III

AN ADJUSTED SET OF MEAN RESONANCE PARAMETER

FOR ^{232}Th IN THE UNRESOLVED RESONANCE REGION

A = 232.0

R = 0.965 $(\text{barn})^{\frac{1}{2}}$ (9) $\gamma_n^{(\ell,J)} = 1$

$\overline{\Gamma}_\gamma^{(\ell,J)}$ = Radiation width, (same for all $\overline{E}$, ℓ and J) = 0.0259 eV (8)

S_o = 0.73 x 10^{-4} (8) $\langle D \rangle^{(1,\frac{3}{2})}$ = 6.475 eV $\langle D \rangle^{(\ell,\frac{1}{2})}$ = 12.95 eV; $\ell = 0$ and 1

Lower Energy keV	Upper Energy keV	S_1 x 10^4	Calculated Values $\langle \sigma_{n\gamma} \rangle$ barns	$\langle \sigma_t \rangle$ barns
3.36	5.54	0.648	1.12	16.45
5.54	9.13	1.34	1.07	15.84
9.13	15.1	1.73	0.98	15.44
15.1	24.8	1.87	0.82	15.18
24.8	40.9	1.23	0.56	14.44

band of values reported by various workers as compiled by the author in Table I. The mean resonance data set given in Table III differs from that given already in ENDF/B-IV for ^{232}Th in the sense that the former reproduces the observed cross sections better than the latter in the various sub-regions of the unresolved resonance energy region.

It must be noted that the energy group structure used in Table III corresponds to the multigroup structure used in fast reactor calculations at our research centre. This energy structure is by no means universal and therefore if a different energy group structure were to be followed for the multigroup cross section set by the reactor designer, these resonance parameters given in Table III cannot be strictly used for the purpose of generation self shielded cross sections since the corresponding average cross sections depend on the choice of the group structure. In other words, the author recommends that not only the evaluation of mean resonance parameters should be carried out in addition to the usual evaluations of cross sections in the unresolved resonance region but also that the evaluations of mean resonance parameters may have to be carried out for the particular multigroup structure used in the reactor calculations. While it may appear that this suggestion of the author is more relevant to that small part of the readership directly concerned with modifying the ENDF/B conventions the following discussion and a comparison of the American ENDF/B system[5] with the German KEDAK[42,43] system will further enlighten the reader on this point.

As already stated in Section 3, from physics point of view, the resonance parameters in the unresolved resonance region stand for the representation of the cross section structure in an energy region. However, the mean resonance parameters themselves vary from one energy region to another. Using statistical formalism, one in fact calculates the mean partial cross sections for the energy region. This energy region is characterized by its mid point $\bar{E}$ in the statistical

formula [See Eq. (2) and Eq. (3)] and by the values of the mean resonance parameters. It is clear, that this energy region should be broad enough to include a number of resonances so as to make the application of statistics precise and at the same time the energy region should be narrow enough so that the mean resonance parameters can be treated as constants within the energy region.

However, we note that in ENDF/B-IV file[5] and in the KEDAK file[42], the mean resonance data is stored as a function of energy point and not as a function of energy region. This apparently contradicts the physics discussed above, where we have stated that there is a histogram of average cross section values and thus of mean resonance data. This means that in both the data files the width of the histogram is considered to be very small; this, however, is an approximation and can be meaningless under certain conditions when the mean cross section shows considerable structure (as is the case for ^{235}U and ^{239}Pu below 10 keV).

Further in ENDF/B processing code, the mean partial cross section at an intermediate point in the unresolved resonance region is calculated by interpolation of the cross section values. In MIGROS-3, the processing code for KEDAK[43], the same is calculated by interpolation of the mean resonance data. In ENDF/B-IV processing code[5], the self shielded cross section at an intermediate point is calculated by interpolation from the calculated self shielded cross sections at the two end points where the mean resonance data are given. But in MIGROS-3, the self shielded cross section is obtained from the mean resonance data which itself if obtained by interpolation of the mean resonance data provided at the end points. The assumption that is implicit in the procedure followed by KEDAK[42] and MIGROS[43] is that the mean resonance parameters vary smoothly in the entire unresolved resonance region.

The procedure followed by MIGROS-3[43] takes much less computing time than the processing method followed in ENDF/B[5] but it must

be stressed that the MIGROS procedure can lead to significant errors when there is a structure in the mean cross sections in the unresolved resonance region (as in the case of fissile isotopes like ^{235}U and ^{239}Pu which exhibit intermediate structures).

The effect of such approximations in the processing of unresolved resonance data on the calculation of self shielded cross sections and on the subsequent calculations of integral parameters of fast power reactors have not however been studied thus far. The calculation of K_{eff} may not itself be much affected by any of these processing methods. However, calculations of second order effects such as the temperature derivatives of self shielded cross sections (which affect the prediction of Doppler Coefficient) in the unresolved resonance region may get affected significantly.

7. COMMENTS ON THE POSSIBILITY OF ADJUSTMENTS OF CROSS SECTIONS THROUGH THE CHOICE OF THE MEAN RESONANCE DATA SET

Let us digress for a while at this point. We note that essentially the role of mean resonance parameters is in calculating the composition and the temperature dependent or the so called self shielded cross sections. These are the cross sections which actually go into the reactor calculations made for predicting the integral parameters including the reactivity coefficients of a fast reactor systems. The self shielded cross section $\tilde{\sigma}_x(\sigma_0, T, \bar{E})$ is given by[21].

$$\tilde{\sigma}_x(\sigma_0, T, \bar{E}) = f_x(\sigma_0, T, \bar{E})\langle\sigma_x\rangle(\bar{E}) \quad (4)$$

where σ_0 stands for the composition, T the temperature and, $\bar{E}$ the average energy of group and f_x is the self shielding factor, which is defined[21] as the ratio of self shielded cross section to infinite dilution cross section $\langle\sigma_x\rangle(\bar{E})$. The suffix x stands to denote the reaction process :- capture, scattering etc. In the adjustment of group cross

sections[22-30] to fit the measured values of integral parameters of a given series of fast reactor assemblies it is usually the infinite dilution cross sections which are adjusted and the self shielding factors have always been left undisturbed. We wish to state here that the possibility of even doing away with the adjustment of infinite dilution cross sections and instead attempting to 'adjust' the self shielding factors to get better agreement between the experimentally obtained and the theoretically predicted values of the various integral parameters, has not been given attention thus far.

The 'adjustment' of self shielding factors is a difficult task as it should not be done directly but rather it should be done by adjusting the set of mean resonance parameters corresponding to given mean cross sections for the energy groups in the unresolved resonance region. Since the self shielding factors as well as their temperature derivatives are different for different sets of mean resonance parameters (all sets, of course leading to the same infinite dilution cross section), it is possible to suggest that suitable choices of the mean resonance parameter sets be made for the various fertile and fissile nuclides in order to get better agreement between theoretical predictions and the experimentally measured values of integral parameters. Theoretically this procedure of adjusting the self shielding factor through the choice of the set of mean resonance parameters is apparently more satisfying since this procedure leaves the evaluated cross sections undisturbed. A mechnism for such adjustments of mean resonance parameter set corresponding to a given recommended fission or capture cross sections in the unresolved resonance region is likely to be very difficult. This is because the mechanism of adjustment for choosing a set of mean resonance parameters depends on the nuclide under consideration. Let us consider the case of ^{235}U as an illustrative example. It was demonstrated by the present author[31] that the evaluated magnitude of the mean fission width for ^{235}U in the unresolved resonance region is strongly

dependent on the assumed value of s wave strength function. Since the reported spread[11,34] in the s wave strength function for ^{235}U is around 30% one can essentially vary the s wave strength function within its quoted uncertainty limits and obtain different sets of mean resonance parameters keeping the infinite dilution cross sections same for all these sets. Since different sets of mean resonance parameters give rise[6] to different values for self shielding factors we can see if a suitable choice of the mean resonance parameter set can remove the discrepancy (or reduce the discrepancy considerably) which exists between theoretically calculated and the experimentally measured values of an integral parameter. This method of adjustment of self shielding factor through the choice of the mean resonance parameter should work well whenever the unresolved resonance region contributes significantly to the integral parameter under consideration. The possibility of adjusting the mean resonance data sets has also been just pointed out by Rowlands et. al[32]. At present, in fact, the calculations made recently at our Centre[33] show that the magnitude of central Doppler worth calculated for the case of ^{235}U sample in ZPR-6-7 assembly can have a spread of about 12% corresponding to the choice of the s wave strength function which is used for the evaluation of mean fission width in the unresolved resonance region. It may be pointed out here that the unresolved region practically covers the entire lower energy region[34] below 50 keV for ^{235}U nuclide. However, this experience with ^{235}U cannot be directly extrapolated to the case of ^{232}Th. The impact of nonuniqueness in the mean resonance data sets for ^{232}Th will be considerably less than that for ^{235}U as the fertile isotope ^{232}Th has a larger resolved resonance region and does not have the fission component, for the Doppler effect.

It is in principle possible to determine average resonance parameters for a nuclide by analysing the thick sample transmission and self indication measurements[35-38] carried out with the sample at different temperatures. Mean resonance parameters determined by this procedure have been reported by Vankov et al[35] and Byoun et. al[36] for

^{238}U isotope. These measurements of average neutron transmission and self indication ratio measurements were performed at various temperatures and sample thicknesses, on depleted uranium, upto 100 keV. Stochastic sampling and analytical methods have been used to interpret these data[36]. According to Byoun et. al[36], the average resonance parameters which fit these data in the unresolved resonance region are in 'essential agreement' with the extrapolation of the resolved resonance region average parameters. While these experiments have shed light on local fluctuation of mean resonance parameters, some theoretical work is required for interpretation of data obtained with thick samples at low temperatures. Direct measurements of self shielding factors for natural iron and ^{23}Na have been reported by Arnaud et. al[38]. In their measurements, a sample of thickness is exposed to a shielded neutron flux which is obtained by transmission through a sample of the same material of thickness X. By measuring the capture rates in the sample of thickness x for various thicknesses X, it is possible to obtain the self shielded cross section and the self shielding factor corresponding to zero background dilution (See Appendix. A). The present author recommends that such measurements be performed for ^{232}Th isotope to increase our confidence in and validate the theoretical procedure for the evaluation of mean resonance parameters. The methods used at present for evaluating mean resonance parameters are not satisfactory because of the limitations inherent in the statistical approach[1-7, 19, 20, 33] and therefore the experiments suggested above will greatly help improve the situation. Alternatively as pointed out in the introduction, the direct use of the Doppler broadened cross sections for ^{232}Th may alleviate the problem to some extent when acceptable high resolution cross section measurements are performed for this nuclide.

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APPENDIX. A

A.1 Definition and Use of Self Shielding Factor

The self shielding factor approach enables the possibility of having a composition independent cross section library. This library can be used many times for various reactor calculations leading to economy in computing time. The theoretical basis is as follows. Now, the effective cross section is given by :

$$\tilde{\sigma}^{i}_{xg} = \frac{\int_{g} dE\ \sigma^{i}_{x}(E)\,\phi(E)}{\int_{g} dE\,\phi(E)} \qquad (A.1.1)$$

Where g : group denoting an energy region (eg. Eg+1)

x : reaction process

i : isotope

E : Energy in g

ϕ : Neutron scalar flux

σ : microscopic cross section

Since, the flux is not known apriori and the intragroup flux is modelled as : $\phi(E) = \frac{W(E)}{\Sigma_t(E)}$ (A.1.2)

Where W(E) is a smooth function of energy, reflecting the fission and scattering sources into E and $\Sigma_t(E)$ is the energy dependent total macroscopic cross section. The reaction rate becomes

$$\int_{g} \frac{\sigma^{i}_{x}(E)\,W(E)\,dE}{\sigma_{p}^{eff} + \sigma_{t}(E)} \qquad (A.1.3)$$

where

$$\sigma_p^{eff} = \frac{1}{N_i} \sum_{d \neq i} N_d \sigma_t^d \qquad \text{(A. 1. 4)}$$

where N_i is the number density for the isotope i in the mixture. The simplification comes from the assumption that σ_p^{eff} is constant within the energy group g. Thus, we can write, dropping the superscript i referring to the isotope for convenience,

$$\tilde{\sigma}_{xg} = \frac{\int_g \frac{\sigma_x}{\sigma_p^{eff} + \sigma_t} W dE}{\int_g \frac{1}{\sigma_p^{eff} + \sigma_t} W dE} \qquad \text{(A. 1.5)}$$

This expression is evaluated for various σ_p^{eff} values and temperatures in the form of self shielding factors f_{xg} and infinite dilution cross section.

$$f_{xg} = \frac{\tilde{\sigma}_{xg}(\sigma_p^{eff}, T)}{\langle \sigma_{xg} \rangle} \qquad \text{(A. 1. 6)}$$

For heterogeneous systems an additional escape cross section is added using equivalence principles. For the reactor composition and temperature, the corresponding self shielded cross sections are obtained by interpolating the f-factors corresponding to its value of σ_p^{eff}

A.2 Characteristics of Self Shielding Factors

Using $\langle \quad \rangle$ to denote the integration over energy we rewrite Eq. (A.1.6) as

$$f_{xg} = \frac{\langle \sigma_x \phi \rangle}{\langle \sigma_x \rangle \langle \phi \rangle} \qquad \text{(A. 2. 1)}$$

where

$$\phi = \left\langle \frac{W(E)}{\sigma_p^{eff} + \sigma_t(E)} \right\rangle \qquad \text{(A.2.2)}$$

With the definition of covariance

$$Cov(a,b) = \langle (a - \langle a \rangle)(b - \langle b \rangle) \rangle \qquad \text{(A.2.3)}$$

We rewrite Eq. (A.2.1) as

$$f_{xg}(\sigma_p^{eff}, T) = 1 + cov\left(\frac{\sigma_x}{\langle \sigma_x \rangle}, \frac{\phi}{\langle \phi \rangle}\right) \qquad \text{(A.2.4)}$$

Whenever σ_x shows a peak, the flux ϕ in general, shows a dip and vice versa. Thus, the covariance is negative and the maximum value of f_{xg} is unity. Further, since, both the fluxes and the cross sections are not negative from physical considerations, the lower limit of f_{xg} is > 0. Thus

$$0 < f_{xg} < 1 \qquad \text{(A.2.5)}$$

Further, the covariance tends to get reduced as T or σ_p^{eff} increases and therefore, the self shielding factor monotonically increases with dilution and/or temperature. i.e.

$$\frac{\partial f_{xg}}{\partial \sigma_p^{eff}} > 0 \; ; \quad \frac{\partial f_{xg}}{\partial T} > 0 \qquad \text{(A.2.6)}$$

However, deviations from the behaviour given by Eq. (A.2.5) and Eq. (A.2.6) can occur when any of the following situations occur.

a) The narrow resonance approximation built in Eq. (A.1.2) can become invalid in the case of broad resonances.

b) The definition of group boundaries can in some instances result in cutting off the edges of the resonances thereby

causing deviations; (or the group itself might have been defined to be too fine to enclose only a part of the resonance !)

c) The windows in the total cross section due to resonance-potential interference minima in the scattering cross section can overcompensate the influence of the peaks in the fission and the capture cross sections on the covariance.

A.3 Semi-Empirical Determination of Self Shielding Factors

The principle behind the experimental determination of self shielded cross sections can be briefly described as follows :

A sample of thickness x is exposed to a shielded neutron flux which has an energy spread defined by the limits E_k and E_{k+1}.

The shielded neutron flux is obtained by transmission through a sample of the same material of thickness X and is given by

$$\phi = \phi_o \, e^{-n\sigma_t X} \qquad \text{(A.3.1)}$$

Let N be the total number of atoms in the sample x and n is the atom number/cm^3 for the samples X and x. For an energy group k, the capture rate in the sample x is

$$CR(\bar{E}_k, X) = \int_{E_k}^{E_{k+1}} N\phi_o \, e^{-n\sigma_t(E)X} \, \sigma_c(E) \, dE \qquad \text{(A.3.2)}$$

The neutron flux transmitted by the sample X can be expressed as

$$\phi_k(\bar{E}_k, X) = \int_{E_k}^{E_{k+1}} \phi_o \, e^{-n\sigma_t(E)X} \, dE \qquad \text{(A.3.3)}$$

For X = O, the incident flux is not self shielded. Thus, we can determine experimentally

$$\sigma_c(E) \quad \text{and} \quad \langle \sigma_c \rangle_k (\bar{E}_k) \qquad \text{(A.3.4)}$$

$\bar{E}_k$ is the average energy of the k and is taken to be the mid point of the group. k.

The experiments are carried out with different thickness of sample X to obtain the values of following integrals

$$Q_1 = \int_0^\infty CR(\bar{E}_k, x)\,dx = \frac{N}{n}\int_{E_k}^{E_{k+1}} \frac{\sigma_c(E)\,\phi_0}{\sigma_t(E)}\,dE \qquad \text{(A. 3. 5)}$$

and

$$Q_2 = \int_0^\infty \phi_k(\bar{E}_k, x)\,dx = \frac{1}{n}\int_{E_k}^{E_{k+1}} \frac{\phi_0}{\sigma_t(E)}\,dE \qquad \text{(A. 3. 6)}$$

We then obtain

$$\tilde{\sigma}_{ck}(\bar{E}_k, \sigma_p^{eff} = o) = \frac{1}{N}\frac{Q_1}{Q_2} \qquad \text{(A. 3. 7)}$$

$$f_{ck}(\bar{E}_k, \sigma_p^{eff} = o) = \tilde{\sigma}_{ck}/\langle \sigma_c \rangle_k \qquad \text{(A. 3. 8)}$$

For other values of σ_p^{eff}, the self shielding factors can be obtained semi-analytically by multiplying $CR(\bar{E}_k, X)$ and $\phi_k(\bar{E}_k, X)$ by $\exp(-n\sigma_p^{eff}X)$

Several corrections are required to be applied to the experimental values; the corrections[38] for instance are to be applied for multiple neutron scattering and resonance self shielding in the sample x, neutron sensitivity of the capture gamma ray detections, effects of the container of the sample and the neutron scattering by air. As pointed in Ref. 33, the uncertainties associated with such direct measurements of self shielded cross sections need to be investigated.