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# Computation of Resonance-Screened Cross Section by the Dorix-Speng System

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BY THE DORIX-SPENG SYSTEM

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ABSTRACT

The report describes a scheme for computation of group cross sections for fast reactors in energy regions where the resonance structure of the cross sections may be dense. A combination of the programmes Dorix and Speng is then used. Dorix calculates group cross sections for each resonance absorber separately. The interaction between resolved resonances in the same isotope is treated using a method described in a separate report. The interaction between correlated and non-correlated resonances in the unresolved region is also considered. By a Dorix calculation we obtain effective microscopic cross sections which are then read in on a library tape. This library contains both point-by-point data and group cross sections and is used in the Speng programme for computation of spectrum and/or macroscopic cross sections. The resonance interaction between different isotopes is computed in Speng by the same method as was used in the Dorix programme for non-correlated unresolved resonances. Consideration is also given to the width of the resonances compared to the energy loss by a neutron colliding with some of the scattering elements.

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## LIST OF CONTENTS

	<u>Page</u>
1. Introduction	3
2. The method used in separation of different resonance effects	5
3. The calculational scheme in Dorix	14
3.1 The energy group lies in the resolved resonance region	14
3.2 The energy group lies in the unresolved resonance region	15
4. The handling of the resonance region in the Speng programme	21
5. Conclusions	24
6. References	26
Appendix A Calculation of the interaction effect between correlated resonances in the unresolved region	28
Appendix B Calculation of the interaction effect between uncorrelated resonances in the unresolved region	30

## 1. INTRODUCTION

In the Dorix-Speng system for calculation of group cross sections there are several simplifying assumptions about the neutron flux which is used for averaging. These simplifications are based on the circumstance that the system is developed for fast reactor calculations. The Speng programme which is a development of Nespcu, [1,2], computes a neutron spectrum in at most 2000 energy points for a finite homogeneous mixture in  $B_1$ -approximation and can use a calculated or a given spectrum to compute macroscopic cross sections. Because the thermal region is a priori assumed to be of no importance, the heterogeneity effects are largest in the resonance region. But within that region we assume that the effect can be accounted for by the approximate equivalence relation from which a "background cross section" can be calculated for a given heterogeneous system, [4]. Thus the problem is equivalent to a homogeneous one.

The heterogeneity effect can, however, in this way only be given for a cross section which is averaged over at least one resonance. Furthermore, 2000 energy points are not sufficient to cover the resonances point-by-point for the heavy elements and not even for some other elements, e.g., copper. Therefore, the Speng programme must also have averaged cross sections as input data and these are then produced by the programme Dorix (Doppler-broadened Resonance Integrals and X-sections). These cross sections are computed as functions of two parameters, namely, the temperature and the "effective potential cross section". But they are also functions of the resonance widths compared to the energy loss by a neutron colliding with any of the scattering elements in the final mixture. According to the intermediate resonance approximation, [5], we have the following expression for the neutron flux:

$$\Phi_{\kappa\lambda}(E) = \left(\frac{1}{E}\right) \frac{\kappa\sigma_m + \lambda\sigma_p}{\kappa\sigma_m + \sigma_a + \lambda\sigma_s} \quad (1.1)$$

This expression is derived under the assumption that the mixture contains only one resonance absorber in the actual energy range. The cor-

responding absorption cross section is  $\sigma_a$ , the scattering cross section is  $\sigma_s$  and the potential cross section is  $\sigma_p$ . The other isotopes are pure scatterers and their resulting cross section per atom of the resonance absorber is  $\sigma_m$ . The parameters,  $\kappa$  and  $\lambda$ , can be determined by assuming isotropic scattering in the laboratory system and knowing the atomic masses for all isotopes. Now, we define an effective potential cross section by the expression

$$\sigma_p^{\text{eff}} = \kappa\sigma_m + \lambda\sigma_p \quad (1.2)$$

But if we introduce Eq. (1.2) into Eq. (1.1), the flux is a function both of  $\sigma_p^{\text{eff}}$  and of  $\lambda$ , separately, and these have different values for different resonances. Therefore, if this expression for the flux is used to calculate group cross sections, these are not univocally determined by  $\sigma_p^{\text{eff}}$ . But we will still use this approach and define an average effective potential cross section as the arithmetical mean value of  $\sigma_p^{\text{eff}}$  over all resonances in a group.

The  $1/E$ -dependence of the flux is only valid for thermal reactors, but Eq. (1.1) can also be applied to fast reactor spectra for narrow energy groups.

The flux given by Eq. (1.1) gives a resonance integral which is a second order approximation to the solution of the slowing down equation with an isolated resonance at zero temperature. It is not shown that the resonance integral divided by the cross section is consistent with a more exact calculation of the flux. We have, however, rather arbitrarily used this approach in Dorix.

It is shown by McKay and Pollard, [19], and by Sehgal, [20], that the parameters  $\kappa$  and  $\lambda$  can be calculated assuming zero temperature and used for a Doppler-broadened case without much loss in accuracy.

The interaction between different resonances is calculated in different ways depending upon the special type of overlapping. One boundary goes between statistically correlated and non-correlated resonances. This division is, however, not strictly maintained for resonances in the same isotope. If these resonances are resolved, it

is not necessary to separate between different  $l$ - and J-values. Further, the division between resolved and unresolved resonances is not maintained in calculating the interaction effect between different isotopes. This effect is calculated in Speng under the usual statistical assumption for non-correlated resonances.

The  $\psi$ - and  $\chi$ -functions which give the shape of the Doppler-broadened resonance cross sections are calculated using the method of O'Shea and Thacher, [6]. The integrals for obtaining J-functions are solved by the Gaussian quadrature in the region where no sufficiently accurate analytical expressions are available. The programming of Dorix was done by B Eriksson [7, 8].

## 2. THE METHOD USED IN SEPARATION OF DIFFERENT RESONANCE EFFECTS

We define a resonance integral of a reaction  $x$ , corresponding to a single resonance,  $k$ , in an isotope,  $i$ , by the following expression:

$$RI_{x, k}^{(i)} = \int_0^{\infty} \phi(E) \sigma_{x, k}^{(i)}(E) dE \quad (2.1)$$

The resonance integral will then have contributions from the whole energy region, but we will assume that it can be concentrated to one single group. The error we introduce by this assumption will, in general, be small because the contribution from one group, say,  $g_1$ , to another group,  $g_2$ , will be small and normally of the same order as the contribution from  $g_2$  to  $g_1$ .

It is useful to define a resonance integral for a given isotope in a given group,  $g$ , by summing  $RI_{x, k}^{(i)}$  over all  $k$  which belong to  $g$ :

$$RI_{x, g}^{(i)} = \sum_k RI_{x, k}^{(i)} \quad (2.2)$$

The corresponding microscopic cross section is then obtained by dividing the resonance integral by the average flux:

$$\bar{\sigma}_{x, g}^{(i)} = \frac{RI_{x, g}^{(i)}}{\int_{\Delta E} \phi(E) dE} \quad (2.3)$$

where  $\Delta E$  is the group width.

As a generalisation of Eq. (1.1), we assume that the flux can be written in the following form:

$$\phi(E) = \frac{1}{E_g^*} \frac{\sigma_{p,i}^{\text{eff}}}{\sigma_{p,i}^{\text{eff}} + \sum_{j,n} \sigma_{r,j,n}} \quad (2.4)$$

$E_g^*$  is an average group energy which will be defined later.  $\sigma_{p,i}^{\text{eff}}$  is obtained by using the intermediate resonance approximation:

$$\sigma_{p,i}^{\text{eff}} = \kappa \left( \sum_m \sigma_{t,m} + \sum_{j \neq i} \sigma_{p,j} \right) + \lambda \sigma_{p,i} \quad (2.5)$$

where  $\sigma_{t,m}$  is the total cross section of the structural material  $m$  which has no resonances in the actual region, and  $\sigma_{p,j}$  is the potential cross section of the resonance absorber  $j$ .  $\sigma_{r,j,n}$  in Eq. (2.4) is a modified resonance cross section for resonance  $n$  in isotope  $j$ , such that the scattering cross section is multiplied by  $\lambda$  according to Eq. (1.1).

We will, for completeness, also give the procedure for calculation of the parameters,  $\kappa$  and  $\lambda$ , in Eq. (2.5). In the unresolved resonance region we set  $\kappa = \lambda = 1$ . In the resolved region they must be labelled according to the resonance index  $k$  of the isotope  $i$ . We start with the calculation of some auxiliary quantities. For every isotope  $i$  in the composition we compute:

$$\alpha_i = \left( \frac{A_i - 1}{A_i + 1} \right)^2 \quad (2.6)$$

and

$$\delta_{i,k} = \left( \frac{2}{\Gamma_k} \right) E_k (1 - \alpha_i) \quad (2.7)$$

where  $A_i$  is the atomic weight,  $\Gamma_k$  is the total resonance width and  $E_k$  the resonance energy. Now, we assume that the resonance  $k$  corresponds to isotope  $i$ , that the resonance absorbers with the isotope indices  $j$  have the potential cross sections  $\sigma_{p,j}$ , and that the structural materials with the isotope indices  $m$  have the total cross sections  $\sigma_{t,m}$ .



All cross sections are given per atom of the isotope  $i$ . Then we calculate an unreduced background cross section from the expression:

$$\sigma_{b,i} = \sum_{j \neq i} \sigma_{p,j} + \sum_m \sigma_{t,m} \quad (2.8)$$

For the resonance  $k$  we also calculate the peak cross section:

$$\sigma_{o,k} = \frac{2.60 \times 10^6}{E_k} g_k \frac{\Gamma_{n,k}}{\Gamma_k} \quad (2.9)$$

where  $g_k$  is the statistical spin factor and  $\Gamma_{n,k}$  is the neutron width.  $E_k$  must then be given in electron volts. Now, as a first trial we set  $\kappa_k = \lambda_k = 1$  and calculate:

$$x_{j,k} = \frac{\delta_{j,k}}{\beta_{1,1} + \beta_{\kappa,\lambda}} \quad (2.10)$$

where

$$\beta_{\kappa,\lambda}^2 = 1 + \frac{\sigma_{o,k}}{\lambda_k \sigma_{p,i} + \kappa_k \sigma_b} \left( \frac{\Gamma_{a,k} + \lambda_k \Gamma_{n,k}}{\Gamma_k} \right) \quad (2.11)$$

$\Gamma_{a,k}$  is the absorption width. New values for  $\lambda_k$  and  $\kappa_k$  are then obtained from the expressions:

$$\lambda_k = 1 - \frac{\text{arc tg } x_{i,k}}{x_{i,k}} \quad (2.12)$$

$$\kappa_k = 1 - \sum_{j \neq i} \frac{\sigma_{p,j}}{\sigma_b} \frac{\text{arc tg } x_{j,k}}{x_{j,k}} - \sum_m \frac{\sigma_{t,m}}{\sigma_b} \frac{\text{arc tg } x_{m,k}}{x_{m,k}} \quad (2.13)$$

Eq:s (2.10) to (2.13) can then be used for an iterative calculation of  $\lambda_k$  and  $\kappa_k$  with arbitrary accuracy.

Now, the flux  $\phi(E)$  should have an index  $k$  because it is a function of  $\lambda_k$  and  $\kappa_k$ . But these quantities are calculated under the assumption that the resonances are well separated. This is not consistent with Eq. (2.4), but we can let  $\sigma_{p,i}^{\text{eff}}$  change abruptly from resonance to resonance and write

$$\phi(E) = \frac{1}{E_g} \frac{\sigma_{p,i}^{\text{eff}}(E)}{\sigma_{p,i}^{\text{eff}}(E) + \sum_{j,n} \sigma_{r,j,n}} \quad (2.14)$$

Then, Eq. (2.1) can be written in the following approximative form:

$$RI_{x,k}^{(i)} = \frac{\sigma_{p,i,k}^{\text{eff}}}{E_g} \int_0^{\infty} \frac{\sigma_{x,k}^{(i)} dE}{\sigma_{p,i,k}^{\text{eff}} + \sum_{j,n} \sigma_{r,j,n}} \quad (2.15)$$

We have then added a new index, k, to the effective potential cross section. Eq. (2.15) is, of course, less accurate in the wings of resonance k where other resonances dominate. The corresponding approximation to the average flux is:

$$\phi = \frac{1}{E_g} \left[ \Delta E - \sum_{i,k} \int_0^{\infty} \frac{\sigma_{r,i,k} dE}{\sigma_{p,i,k}^{\text{eff}} + \sum_{j,n} \sigma_{r,j,n}} \right] \quad (2.16)$$

The equations above involve interaction between different resonances. The method we have adopted to calculate this effect explicitly is developed by Fischer, [9], but was originally given by Rowlands, [21]. The effective cross section can then be written in the following form, [3]:

$$\bar{\sigma}_{x,g}^{(i)} = \frac{\sum_k \left( \frac{\Gamma_k}{\lambda_k \Gamma_{n,k} + \Gamma_{a,k}} \right) \sigma_{p,i,k}^{\text{eff}} \Gamma_{x,k} \left\{ J(\theta_k, \beta_k) + \sum_{j, l \neq k} \left[ F_1(\beta_k, \beta_l) - F_2(\beta_k, \beta_l) \right] \right\}}{\Delta E - \sum_{j,k} \Gamma_k \left[ J(\theta_k, \beta_k) + \sum_{l \neq k} F_1(\beta_k, \beta_l) \right]} \quad (2.17)$$

Here,

$$J(\theta_k, \beta_k) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(x, \theta_k) dx}{\psi(x, \theta_k) + \chi(x, \theta_k) \text{tg } 2\delta_i + \beta_k} \quad (2.18)$$

where  $\psi$  and  $\chi$  are the symmetric and antisymmetric resonance line shape functions,

$$\theta_k = \frac{\Gamma_k}{\sqrt{\frac{4kTE_k}{A_i}}} \quad (2.19)$$

$$\delta_i = \frac{R_i}{2\lambda_k} \quad (2.20)$$

$$R_i = \sqrt{\frac{\sigma_{p,i}}{4\pi}} \quad (2.21)$$

$$\lambda_k = 10^3 \sqrt{\frac{2.60}{4\pi E_k}} \quad (2.22)$$

and

$$\beta_k = \frac{\sigma_{p,i,k}^{\text{eff}}}{\sigma_{o,k} \cos 2\delta_i} \left( \frac{\Gamma_k}{\lambda_k \Gamma_{n,k} + \Gamma_{a,k}} \right) \quad (2.23)$$

$E_k$  must be given in electron volts and  $\sigma_{p,i}$  in barns.  $\sigma_{o,k}$  is obtained from Eq. (2.9). The functions  $F_1(\beta_k, \beta_l)$  and  $F_2(\beta_k, \beta_l)$  give the resonance interaction effect and are obtained from the expressions:

$$F_1(\beta_k, \beta_l) = \frac{\beta_k}{2} \int_{-\infty}^{\infty} \frac{\delta}{\delta\beta_k} \left( \frac{\psi_k}{\psi_k + \beta_k} \right) \left( \frac{\beta_l}{\psi_l + \beta_l} \right) dx \quad (2.24)$$

$$F_2(\beta_k, \beta_l) = \frac{1}{2} \int_{-\infty}^{\infty} \left[ \frac{\psi_k}{\psi_k + \beta_k} + \beta_k \frac{\delta}{\delta\beta_k} \left( \frac{\psi_k}{\psi_k + \beta_k} \right) \right] \cdot \left[ \frac{\psi_l}{\psi_l + \beta_l} + \beta_l \frac{\delta}{\delta\beta_l} \left( \frac{\psi_l}{\psi_l + \beta_l} \right) \right] \quad (2.25)$$

In Eq. (2.17) the indices  $i$  and  $k$  are coupled together so that to each isotope index  $i$  there corresponds a series of  $k$ -values. The  $l$ -values in numerator and denominator as well as the  $k$ -values in the denominator run over all isotope indices  $j$ . It is now convenient to separate out the quantities which belong to the isotope  $i$ . For compactness, we then write Eq. (2.17) in the following form:

$$\bar{\sigma}_{x,g}^{(i)} = \left[ \frac{\bar{\sigma}_{x,g,o}^{(i)} - \bar{\sigma}_{x,g,i}^{(i)}}{1 - \langle A_i \rangle} \right] \left\{ 1 + \frac{\sum_{j \neq i} \left[ \langle A_j \rangle - \frac{\bar{\sigma}_{x,g,j}^{(i)} (1 - \langle A_i \rangle)}{\bar{\sigma}_{x,g,o}^{(i)} - \bar{\sigma}_{x,g,i}^{(i)}} \right]}{1 - \langle A_i \rangle - \sum_{j \neq i} \langle A_j \rangle} \right\} \quad (2.26)$$

where

$$\bar{\sigma}_{x,g,o}^{(i)} = \frac{1}{\Delta E} \sum_k \left( \frac{\Gamma_k}{\lambda \Gamma_{n,k} + \Gamma_{a,k}} \right) \sigma_{p,i,k}^{\text{eff}} \Gamma_{x,k} J(\theta_k, \beta_k) \quad (2.27)$$

$$\begin{aligned} \bar{\sigma}_{x,g,j}^{(i)} &= \frac{-1}{\Delta E} \sum_{k \neq i} \left( \frac{\Gamma_k}{\lambda \Gamma_{n,k} + \Gamma_{a,k}} \right) \sigma_{p,i,k}^{\text{eff}} \Gamma_{x,k} \sum_{\ell \neq j} \cdot \\ &\cdot \left[ F_1(\beta_k, \beta_\ell) - F_2(\beta_k, \beta_\ell) \right] \end{aligned} \quad (2.28)$$

$$\langle A_j \rangle = \frac{1}{\Delta E} \sum_{k \neq j} \Gamma_k \left[ J(\theta_k, \beta_k) + \sum_{\ell \neq k} F_1(\beta_k, \beta_\ell) \right] \quad (2.29)$$

Skew brackets indicate here and in what follows that the enclosed quantity is an average value.

In Eq:s (2.28) and (2.29), the symbols of type  $k \neq i$  mean that the resonance index  $k$  corresponds to an isotope index  $i$ .

The first bracket expression on the r. h. s. of Eq. (2.26) is computed in Dorix and the rest in Speng. The quantity  $\bar{\sigma}_{x,g,i}^{(i)}$  contributes to the interaction effect between resonances of the same isotope but can partly belong to non-correlated resonances. This is taken care of in the unresolved resonance region. In the resolved resonance region the function  $F_1$  is calculated by using a rational approximation to the  $\psi$ -function, [3]. It is found that the usual Gaussian approximation is not appropriate in this region. The integral in Eq. (2.24) is solved analytically and the solution is given in Ref. [3]. The function  $F_2$  which is small to the second order is neglected for correlated resonances but can be calculated in the same way as  $F_1$ . It is shown in Ref. [3] that it is negligible in the resolved regions of the  $^{238}\text{U}$  and  $^{239}\text{Pu}$  resonances.

In the unresolved resonance region we must consider different resonance series', s, separately. For brevity, we omit the group index g in the individual terms of the overlap effect on the resonance integral:

$$\bar{\sigma}_{x, g, i}^{(i)} = \sum_s \langle \sigma_{x, i, s}^{(i)} \rangle \quad (2.30)$$

Then, we write each term in two parts which give the contribution from correlated and non-correlated resonances, respectively:

$$\langle \bar{\sigma}_{x, i, s}^{(i)} \rangle = \langle \sigma_{x, i, s, \text{corr}}^{(i)} \rangle + \langle \sigma_{x, i, s, \text{indep}}^{(i)} \rangle \quad (2.31)$$

The first term on the r.h.s. of Eq. (2.31) is calculated using a first order approximation given by Froelich, [10]. The second term can be written, [3, 9]:

$$\begin{aligned} \langle \sigma_{x, i, s, \text{indep}}^{(i)} \rangle = & \sigma_{p, i}^{\text{eff}} \left\{ \frac{\langle \Gamma_x^{(s)}(J_s - J_s^*) \rangle}{\bar{D}_s} \sum_{t \neq s} \frac{\langle \Gamma(t)_{J_t} \rangle}{\bar{D}_t} + \right. \\ & \left. + \frac{\langle \Gamma^{(s)}_{J_s^*} \rangle}{\bar{D}_s} \sum_{t \neq s} \frac{\langle \Gamma(t)_{J_t^*} \rangle}{\bar{D}_t} \right\} \end{aligned} \quad (2.32)$$

where

$$J_s^* = J_s + \beta_s \frac{\delta J_s}{\delta \beta_s} \quad (2.33)$$

$\beta_s$  is some  $\beta_k$  for the resonance series s.  $\Gamma^{(s)}$  and  $\Gamma_x^{(s)}$  are corresponding resonance widths.  $\bar{D}_s$  is the average spacing between these resonances. The narrow-resonance approximation is used in this region.

The quantity  $\langle A_i \rangle$  in Eq. (2.26) gives the deviation of the average neutron flux from the  $1/E$  dependence. The largest part of it is proportional to the zero order resonance integral. The rest consists of interaction terms and can be separated into one part coming from correlated and another from non-correlated resonances. We then obtain:

$$\langle A_i \rangle = \sum_s \left\{ \frac{\langle \Gamma^{(s)}_{J_s} \rangle}{\bar{D}_s} - \langle a_{i,s} \rangle - \frac{\langle \Gamma^{(J_s - J_s^*)} \rangle}{\bar{D}_s} \sum_{t \neq s} \frac{\langle \Gamma^{(t)}_{J_t} \rangle}{\bar{D}_t} \right\} \quad (2.34)$$

$\langle a_{i,s} \rangle$  is the correlated part of the interaction terms and is calculated using the method given by Froelich, [10]. Using Eq:s (2.30) to (2.34) we then obtain for the single-isotope cross section the following expression with an accuracy of second order:

$$\begin{aligned} \langle \sigma_{x,g}^{(i)} \rangle &= \frac{\langle \bar{\sigma}_{x,g,o}^{(i)} \rangle - \langle \bar{\sigma}_{x,g,i}^{(i)} \rangle}{1 - \langle A_i \rangle} = \\ &= \sigma_{p,i}^{\text{eff}} \sum_s \left\{ \frac{\frac{\langle \Gamma_x^{(s)}_{J_s} \rangle}{\bar{D}_s} - \frac{\langle \sigma_{x,i,s,\text{corr}}^{(i)} \rangle}{\sigma_{p,i}^{\text{eff}}} + \frac{\langle \Gamma_x^{(s)}_{J_s} \rangle}{\bar{D}_s} \sum_{t \neq s} \frac{\langle \Gamma_t^{(J_t - J_t^*)} \rangle}{\bar{D}_t}}{1 + \langle a_{i,s} \rangle - \frac{\langle \Gamma^{(s)}_{J_s} \rangle}{\bar{D}_s} \left[ 1 + \sum_{t \neq s} \frac{\langle \Gamma^{(t)}_{J_t} \rangle}{\bar{D}_t} \right] + \sum_{p \neq s} \frac{\langle \Gamma^{(p)}_{J_p} \rangle}{\bar{D}_p} \sum_{q \neq p} \frac{\langle \Gamma^{(q)}_{(J_q - J_q^*)} \rangle}{\bar{D}_q}} \right\} \end{aligned} \quad (2.35)$$

Eq. (2.35) contains more terms than those given by Fischer, [9]. Because  $J^*$  need not be much smaller than  $J$ , no terms in the equation can be considered to be of higher order than the second. An approximate formula for the interdependence between  $J$  and  $J^*$  is given in appendix B.

The cross sections  $\langle \sigma_{x,g}^{(i)} \rangle$  are given on a library tape which serves as a data tape for the Speng programme. The parameters are  $\sigma_{p,i}^{\text{eff}}$  and the temperature. But, as we have seen,  $\sigma_{p,i}^{\text{eff}}$  is in the resolved resonance region different for each resonance,  $k$ . The parameter we use for the library tape is the arithmetic average for the group.

In order to calculate spectrum and macroscopic cross sections for a given composition, an interpolation between the tabulated values is made by Speng. The interpolated cross sections correspond to the actual  $\sigma_{p,i}^{\text{eff}}$  and temperature. The interpolation formulae are given in section 4. Now,  $\langle \sigma_{x,g}^{(i)} \rangle$  may be multiplied by the correction factor given by the second bracketed expression in Eq. (2.26), in order

to obtain  $\bar{\sigma}_{x,g}^{(i)}$ . This computation is optional because the correction factor is close to 1. It may be expressed in a more elaborate way by inserting the statistical averages of the quantities which enter into Eq. (2.26). For  $\bar{\sigma}_{x,g,j}^{(i)}$  and  $\langle A_j \rangle$  we use Eq:s (2.30) to (2.34), considering that there is no statistical correlation between the isotopes  $i$  and  $j$ . Therefore, if we neglect the interaction between resonances in the same isotope and introduce average values which are summed over the resonance series within an isotope, we obtain for the interaction-corrected cross section a formula which is analogous to Eq. (2.35):

$$\bar{\sigma}_{x,g}^{(i)} = \sigma_{p,i}^{\text{eff}} \frac{\frac{\langle \Gamma_{x,i} J_i \rangle}{\bar{D}_i} + \frac{\langle \Gamma_{x,i} J_i^* \rangle}{\bar{D}_i} \sum_{j \neq i} \frac{\langle \Gamma_j (J_j - J_j^*) \rangle}{\bar{D}_j}}{1 - \frac{\langle \Gamma_i J_i \rangle}{\bar{D}_i} \left[ 1 + \sum_{j \neq i} \frac{\langle \Gamma_j J_j \rangle}{\bar{D}_j} \right] + \sum_{j \neq i} \frac{\langle \Gamma_j J_j \rangle}{\bar{D}_j} \sum_{k \neq j} \frac{\langle \Gamma_k (J_k - J_k^*) \rangle}{\bar{D}_k}}$$

(2.36)

Here, the indices  $i$ ,  $j$ , and  $k$  correspond each to an isotope. For brevity, we introduce the following quantities:

$$h_i = \frac{\langle \Gamma_i J_i \rangle}{\bar{D}_i} \tag{2.37}$$

$$h_i^* = \frac{\langle \Gamma_i J_i^* \rangle}{\bar{D}_i} \tag{2.38}$$

Further, for the quantities of higher than zero order we assume that an average of a product is equal to the product of the averages of each factor. Then, neglecting the interaction within an isotope:

$$\frac{\langle \Gamma_{x,i} J_i^* \rangle}{\bar{D}_i} = \frac{h_i^*}{h_i} \frac{\langle \sigma_{x,g}^{(i)} \rangle}{\sigma_{p,i}^{\text{eff}}} (1 - h_i) \tag{2.39}$$

where

$$\langle \sigma_{x,g}^{(i)} \rangle = \frac{\sigma_{p,i}^{eff} \frac{\langle \Gamma_{x,i} J_i \rangle}{\bar{D}_i}}{1 - h_i} \quad (2.40)$$

From Eq:s (2.36) to (2.40) we then obtain:

$$\bar{\sigma}_{x,g}^{(i)} = \langle \sigma_{x,g}^{(i)} \rangle \frac{(1 - h_i) \left[ 1 + \frac{h_i}{h_i} \sum_{j \neq i}^* (h_j - h_j^*) \right]}{1 - h_i (1 + \sum_{j \neq i}^* h_j) + \sum_{j \neq i}^* h_j \sum_{k \neq j}^* (h_k - h_k^*)} \quad (2.41)$$

Eq. (2.41) is strictly valid only if we neglect the interaction within an isotope but we assume that it is sufficiently accurate even if this interaction is present. Then, for  $\langle \sigma_{x,g}^{(i)} \rangle$  we use the cross sections which are obtained from Eq. (2.35) and tabulated in the Speng library. The quantities  $h$  and  $h^*$  with different subscripts are computed using the formulae in appendix B.

Heterogeneity effects in the resonance region are considered by modifying  $\sigma_{x,g}^{eff}$  according to the equivalence principle. The "shadowing effect" is considered by using the Dancoff correction. The formulae are introduced in the Speng programme by K. Jirlow and K Nyman, [2], and are identical with those given by Hummel et al., [11].

### 3. THE CALCULATIONAL SCHEME IN DORIX

#### 3.1 The energy group lies in the resolved resonance region

We want to obtain cross sections for a resonance absorber,  $i$ , for different temperatures,  $T$ , and for different values of the parameter  $\sigma_{p,i}^{eff}$ . After that the input data are read in, the latter quantity is computed using Eq:s (2.5) to (2.13). But in this case,  $\sigma_{p,j}$  for  $j \neq i$  is substituted by an equally large  $\sigma_{t,m}$  because all other resonance absorbers are neglected. The composition is in other respects chosen to be representative for the type of problem we want to study.

In parallel with the screened cross sections we also compute the cross sections for infinite dilution in order to obtain the screening factors. These cross sections are given by the following expression:



$$\bar{\sigma}_{x, g, \text{inf}}^{(i)} = \frac{\pi}{2} \frac{1}{\Delta E} \sum_k \Gamma_{x, k} \sigma_{o, k} \quad (3.1)$$

where  $\sigma_{o, k}$  is obtained from Eq. (2.9). The screening factor is defined as the ratio between the screened cross section and  $\bar{\sigma}_{x, g, \text{inf}}^{(i)}$ .

The computation of screened cross sections begins with determining the interaction between the resonances in first order approximation. This is given by the function:

$$SU_{x, i} = \sum_k \sigma_{p, i, k}^{\text{eff}} \Gamma_{x, k} \sum_{l \neq k} F_1(\beta_k, \beta_l) \quad (3.2)$$

where  $F_1(\beta_k, \beta_l)$  is defined in Eq. (2.24). The method for calculating this function is given in Ref. [3].

The zero order single resonance integral is

$$RI_{x, k, o}^{(i)} = \frac{\sigma_{p, i, k}^{\text{eff}}}{E_g^*} \Gamma_{x, k} \frac{\Gamma_k}{\lambda_k \Gamma_{n, k} + \Gamma_{a, k}} J(\theta_k, \beta_k) \quad (3.3)$$

where the J-function is defined in Eq. (2.18) and  $E_g^*$  is the mean energy, defined rather arbitrarily (see next section). The main part of the J-function is computed by a Gaussian quadrature but the contributions from large x-values are obtained from analytical approximations, [7]. The  $\psi$ - and  $\chi$ -functions are obtained from the continuous fraction approximation, [6].

The effective cross section is now computed from Eq. (2.17), neglecting the second order overlap effect in the numerator,  $F_2(\beta_k, \beta_l)$ . There is no reason to neglect the second order term in the denominator because it changes the cross section in the same (negative) direction as  $F_2$ .

### 3.2 The energy group lies in the unresolved resonance region

In the unresolved resonance region we assume that the resonances are infinitely narrow. Thus, calculating  $\sigma_{p, i}^{\text{eff}}$  from Eq. (2.5), we assume that  $\kappa = \lambda = 1$ .

The cross sections for infinite dilution are for the resonance series s:

$$\bar{\sigma}_{x, g, \text{inf}}^{(i, s)} = \frac{\pi^2 \lambda_g^2 g^{(s)}}{\bar{D}(s)} S_x^{(s)} \frac{\bar{\Gamma}_n^{(s)} \bar{\Gamma}_x^{(s)}}{\bar{\Gamma}(s)} \quad (3.4)$$

where

$$S_x^{(s)} = \frac{\left\langle \frac{\bar{\Gamma}_n^{(s)} \bar{\Gamma}_x^{(s)}}{\bar{\Gamma}(s)} \right\rangle}{\left( \frac{\bar{\Gamma}_n^{(s)} \bar{\Gamma}_x^{(s)}}{\bar{\Gamma}(s)} \right)} \quad (3.5)$$

The bars over the resonance parameters indicate as do the skew brackets around the products, average values of the respective quantities. The index s is a function of the  $\ell$ -value and the total spin, J. The statistical weight,  $g^{(s)}$  is obtained from the expression

$$g^{(s)} = \frac{2J+1}{2(2I+1)} \quad (3.6)$$

where I is the internal spin factor.

When g occurs as a subscript, it is a group index.

$\lambda_g$  is calculated according to Eq. (2.22) where  $E_k$  is substituted by a mean group energy,  $E_g^*$ . This can be calculated in two ways which are optional:

$$E_g^* = \frac{E_g + E_{g-1}}{2} \quad (3.7)$$

or

$$E_g^* = \sqrt{E_g E_{g-1}} \quad (3.8)$$

where  $E_g$  is the lower energy boundary of the group. The Doppler temperature parameter,  $\theta$ , is calculated from Eq. (2.19) using  $E_g^*$  instead of  $E_k$ .

Eq. (2.20) for the quantum mechanical phase shift can be generalised to consider both s- and p-waves by the following formula, [10]:

$$\delta_{i, l} = \frac{1}{2} \left( \frac{R_i}{\lambda_g} - l \operatorname{arctg} \frac{R_i}{\lambda_g} \right) \quad (3.9)$$

where  $l = 0$  or  $1$ .

The mean distance between the resonances is assumed to be dependent upon the total spin,  $J$ , and the energy in the following way, [10]:

$$\overline{D}^{(s)} = \overline{D}_{J, l} = \frac{D_{0, l}}{2J+1} F_e \quad (3.10)$$

where

$$F_e = \frac{(5 + E_g^* \times 10^{-6})^2}{25} \exp \left[ - \left( \sqrt{89.7(5 - E_g^* \times 10^{-6})} - \sqrt{448.5} \right) \right] \quad (3.11)$$

$\overline{D}_{0, l}$  is the mean distance if  $J=0$  and  $E_g^* = 0$ . For the mean neutron width we use the same formula as in the Eric 2 programme, [12]:

$$\overline{\Gamma}_n^{(s)} = (SF)_l \overline{D}^{(s)} \sqrt{E_g^*} \nu_{l, J} \mu_{l, J}^{(i)} \quad (3.12)$$

where  $(SF)_l$  is the strength function, and

$$\nu_l = \begin{cases} 1 & \text{for } l = 0 \\ \frac{y^2}{1+y^2} & \text{for } l = 1 \end{cases} \quad (3.13)$$

$$y = 0.00191 \sqrt{E_g^*} \quad (3.14)$$

$\mu_{l, j}$  is a weight function and  $= 1$  for  $l = 0$  but may be an integer  $> 1$  for  $l > 0$ .

The functions  $S_x^{(s)}$ , defined by Eq. (3.5) are calculated from formulae which depend upon whether the material is fissile or not. For brevity, we introduce the following quantities:

$$a_1 = 1 + \frac{\bar{\Gamma}_n(s) + \bar{\Gamma}_f(s)}{\Gamma_Y(s)} \quad (3.15)$$

$$a_2 = \frac{2\bar{\Gamma}_n(s)}{\Gamma_Y(s)} \quad (3.16)$$

$$a_3 = \frac{2\bar{\Gamma}_f(s)}{\nu_f \Gamma_Y(s)} \quad (3.17)$$

We assume  $\chi_{\nu}^2$ -distributions for  $\Gamma_x(s)$  where  $x$  corresponds to  $(n, n)$  or  $(n, f)$  reactions.  $\nu_x$  is the number of degrees of freedom in the reaction  $x$ . We also assume that  $\Gamma_Y(s)$  is constant and that  $\nu_n = 1$ . Under these conditions, Klahr and Certain, [13, 14], have shown that the functions  $S_x(s)$  can be written in the following form which is valid both for fissile and for non-fissile isotopes:

$$S_n(s) = 3 a_1 \int_0^{\infty} (1 + a_2 x)^{-2.5} (1 + a_3 x)^{-\frac{\nu_f}{2}} e^{-x} dx \quad (3.18)$$

$$S_Y(s) = a_1 \int_0^{\infty} (1 + a_2 x)^{-1.5} (1 + a_3 x)^{-\frac{\nu_f}{2}} e^{-x} dx \quad (3.19)$$

$$S_f(s) = a_1 \int_0^{\infty} (1 + a_2 x)^{-1.5} (1 + a_3 x)^{-\left(\frac{\nu_f}{2} + 1\right)} e^{-x} dx \quad (3.20)$$

For non-fissile materials, these equations can be partially solved, and we obtain:

$$S_n(s) = \frac{\Gamma_Y(s) + \bar{\Gamma}_n(s) - \Gamma_Y(s) S_Y(s)}{\bar{\Gamma}_n(s)} \quad (3.21)$$

and

$$S_Y(s) = \frac{\Gamma_Y(s) + \bar{\Gamma}_n(s)}{\bar{\Gamma}_n(s)} \left[ 1 - a \sqrt{\pi} e^{a^2} \left( 1 - \frac{2}{\sqrt{\pi}} \int_0^a e^{-y^2} dy \right) \right] \quad (3.22)$$

where

$$a = \sqrt{\frac{\Gamma_Y(s)}{2\Gamma_n(s)}} \quad (3.23)$$

The numerical computation method of the functions  $S_x^{(s)}$  is described in Ref. [8].

For calculation of the J-functions and resonance integrals we take samples of  $\Gamma_n$ - and  $\Gamma_f$ -values in the same way as in the Eric 2 programme, [12]:

$$\Gamma_{n,k}^{(s)} = x_k \bar{\Gamma}_n^{(s)} \quad (3.24)$$

$$\Gamma_{f,q}^{(s)} = y_q \bar{\Gamma}_f^{(s)} \quad (3.25)$$

Assuming a  $\chi_\nu^2$  statistical distribution and that the maximum numbers of the factors  $x_k$  and  $y_q$  are  $N_k$  and  $N_q$ , respectively, we first chose  $N_k - 1$  points,  $z_k$ , on the abscissa of this function so that

$$\int_{z_{k-1}}^{z_k} \chi_\nu^2(x) dx = \frac{1}{N_k} \quad (3.26)$$

The points  $x_k$  are then assumed to be positioned at the "center of gravity" of each partial surface. Then,

$$x_k = N_k \int_{z_{k-1}}^{z_k} x \chi_\nu^2(x) dx \quad (3.27)$$

Eq:s (3.26) and (3.27) are of course also valid for the points  $y_q$  if  $N_k$  is substituted by  $N_q$ . This method was first used by Ferziger et al., [15].

The total resonance width is then also a function of  $k$  and  $q$  and we calculate a corresponding peak resonance cross section for series  $s$ :

$$\sigma_{o,k,q}^{(s)} = 4\pi\lambda_g^2 g^{(s)} \frac{\Gamma_{n,k}^{(s)}}{\Gamma_{k,q}^{(s)}} \cos 2\delta_{i,\ell} \quad (3.28)$$

The J-function can then be computed in the same way as in the resolved resonance region for  $N_k \cdot N_q$  values of  $\theta_{k,q}$  and  $\beta_{k,q}^{(s)}$ , where

$$\beta_{k,q}^{(s)} = \frac{\sigma_{p,i}^{eff}}{\sigma_{o,k,q}^{(s)}} \quad (3.29)$$

However, in order to save time, this method is normally only used for one s-value, namely, for that which has the highest probability to give the largest contribution to the cross section. This s-value corresponds to  $\ell = 0$  and the largest spin-value because  $g^{(s)}$  is then largest and  $\overline{D}^{(s)}$  smallest. For other resonance series, the J-function is normally computed by the approximation given by Doherty, [12, 16]. The more accurate method given in Ref. [7] can be chosen for these s-values as an option.

The zero order resonance integral is then:

$$RI_{x,o}^{(i,s)} = \frac{\sigma_{p,i}^{eff}}{E_g} \frac{\langle \Gamma_x^{(s)} J(\theta, \beta^{(s)}) \rangle}{\overline{D}^{(s)}} \quad (3.30)$$

where

$$\langle \Gamma_x^{(s)} J(\theta, \beta^{(s)}) \rangle = \frac{1}{N_k N_q} \sum_{k=1}^{N_k} \sum_{q=1}^{N_q} \overline{\Gamma}_x^{(s)} J(\theta_{k,q}, \beta_{k,q}^{(s)}) \quad (3.31)$$

In the calculation of the interaction effect between resonances in the same series we follow Froelich, [10]. According to Eq. (2.35), this effect is given by the quantities  $\langle \sigma_{x,i,s,corr}^{(i)} \rangle$  and  $\langle a_{i,s} \rangle$ . The formulae for calculation of these quantities are given in appendix A, Eq:s (A.11) and (A.12).

The interaction effect between different resonance series is given by quantities of the type  $\langle \Gamma J \rangle / D$  and  $\langle \Gamma J^* \rangle / D$ . The accuracy of these need not be very good and it is not necessary to calculate the J-functions involved by any of the methods we have mentioned earlier. The method we use in Dorix for calculating these quantities is described

in Appendix B. Comparative computations have been performed using this and more accurate methods, [17]. The interaction was then calculated between resolved resonances in  $^{238}\text{U}$  and  $^{239}\text{Pu}$  below 250 keV. The conclusion was that the method of calculation of  $\langle \Gamma J \rangle / D$  and  $\langle \Gamma J^* \rangle / D$  described in Appendix B causes errors of less than 30 % in most cases. The statistical assumption about infinitely large samples caused, however, much larger errors in this energy region. The group widths were then of the order of 20 to 30 eV.

We have now all quantities needed to calculate the single-isotope cross sections from Eq. (2.35). The computer programme is written in Fortran 4 language.

#### 4. THE HANDLING OF THE RESONANCE REGION IN THE SPENG PROGRAMME

The theoretical basis for the Speng programme is given in Ref. [1]. A specific feature of Speng is the very flexible mesh of energy points for the data tabulation and for the computations. The programming was done by K Nyman [2]. Contributions to the content have also been made by K Jirlow.

The Speng data library contains screened resonance cross sections together with smooth cross sections and other data necessary for fast reactor calculations. The number of temperatures and the number of effective potential cross sections can differ from group to group and they are therefore given before every group.

For the solution of a problem, the Speng programme needs cross sections for a composition and a temperature which are given in the input data. The programme must therefore compute an effective potential cross section. For a homogeneous mixture this is made using Eq. (2.5). For a heterogeneous composition we have two alternatives. One is that we have a single foil or lump surrounded by a homogeneous scattering medium. The composition determining  $\sigma_{p,i}^{\text{eff}}$  is then that of the lump together with the collision chord in the lump. Thus,

$$\sigma_{p,i}^{\text{eff}} = \sigma_{p,i,\text{homog}}^{\text{eff}} + \frac{1}{N_i \bar{\ell}} \quad (4.1)$$

where  $\sigma_{p,i,\text{homog}}^{\text{eff}}$  is calculated for the lump from Eq. (2.5),  $N_i$  is the atomic density of isotope  $i$  and  $\bar{\lambda}$  is the collision chord in the lump. The other alternative is that the composition consists of a lattice of two components. Only one of them which we call the fuel can contain resonance absorbers. Then, following Hummel et al., [11],

$$\sigma_{p,i}^{\text{eff}} = \sigma_{p,i,\text{homog}}^{\text{eff}} + \frac{v_{\text{fuel}}}{N_i \bar{\lambda}} \cdot \frac{a\gamma(E)}{1 + (a-1)(1-\gamma(E))} \quad (4.2)$$

where  $\sigma_{p,i,\text{homog}}^{\text{eff}}$  is calculated for the fuel. The quantity  $v_{\text{fuel}}$  is the fuel volume fraction of the total mixture. The constant  $a$  which for fast reactors is usually chosen to be of the order 1.2 to 1.5, [11], is given in the input data.  $\gamma(E)$  is computed by the programme assuming either slab or cylindrical geometry.

If the neutron spectrum is to be calculated, the programme integrates the slowing down equation in  $B_1$ -approximation. The density of the energy points used in this integration is normally given by the largest tabulation density at the given energy of any isotope in the composition. But the density can be influenced by the input data because maximum and minimum step lengths are given along the integration interval. These step lengths can change at arbitrary points. Thus, if the maximum step length is smaller than any tabulation interval of the cross sections, the integration step length is determined by the given maximum step length. This is especially worth while in the resonance region where the cross sections may change by several orders of magnitude between neighbouring groups.

If the problem involves calculation of macroscopic cross sections, the programme computes the average values using a given neutron spectrum as weight function. The energy points used in the integration are then normally those of the neutron spectrum and of the energy points of all tabulated cross sections. These cross sections are assumed to vary linearly from point to point if they are defined as "smooth" cross sections. They describe of course a histogramme if they are given as screened resonance cross sections. Also, if the directive INVERSE is not given, the flux is assumed either to vary



linearly or to describe a histogramme between the tabulated points. But if this directive is given, the flux is assumed to vary as the inverse of the total macroscopic cross section between these points. The macroscopic cross section is then given at intervals which are 2/3 of the interval of the most densely tabulated cross sections in a region determined by the programme which includes the actual flux interval.

In all these cases, we must first determine the screened resonance cross sections for every resonance absorber  $i$  in those energy groups that are tabulated for isotope  $i$ . The effective potential cross sections must then also be calculated for these groups. The cross sections for the "background" isotopes are hereby obtained from the data given in arbitrary points by averaging with a constant weight function.

The interpolation in the data library between the tabulated temperatures and effective potential cross sections is based on rather arbitrary formulae. The cross section as a function of the temperature is given by the expression

$$\bar{\sigma}_{x,g}^{(i)}(T) = A + \frac{B}{T} \quad (4.3)$$

The dependence on the effective potential cross section is assumed to be:

$$\bar{\sigma}_{x,g}^{(i)}(\sigma_{p,i}^{\text{eff}}) = \bar{\sigma}_{x,g}^{(i)}(\infty) \sqrt{\frac{a + \sigma_{p,i}^{\text{eff}}}{b + \sigma_{p,i}^{\text{eff}}}} \quad (4.4)$$

The advantage with these formulae compared to linear interpolation is that the second derivatives of the respective functions have the same sign as the second derivatives of smooth curves through calculated values of the cross section as a function of  $T$  and  $\sigma_{p,i}^{\text{eff}}$ .

When the cross sections for a mixture are computed, a correction for the resonance interaction between different isotopes is made if the directive INTERACTION is given. This effect is then obtained from Eq. (2.41). The functions  $h_j$  and  $h_j^*$  for all resonance absorbers

$j$  are calculated using the method given in Appendix B. It should be noticed that this method has theoretical validity only if the statistical samples are infinitely large. This is not the case for the narrow energy groups used in the Speng library. Therefore, the interaction effect in the single groups will not be calculated correctly, especially in the low energy groups, say, below 500 eV. But the average interaction effect over the whole resonance region is assumed to have a much higher accuracy than the effect in the single groups. An investigation of errors introduced by the statistical assumption and by the approximation of  $h_j^*$  we have used is made in Ref. [17].

The Speng programme calculates the neutron spectrum and the macroscopic cross sections assuming a homogeneous mixture of the microscopic cross sections which we have now obtained. In order to take into consideration an eventual heterogeneity, group cross sections for different zones must be calculated separately and the groupdependent transport equation is to be solved for the specific micro-structure. But one should then consider carefully the limitations of the fundamental mode approximation.

## 5. CONCLUSIONS

The conditions under which the Dorix-Speng system was developed were limited personnel and computing machine resources, so that all the problems involved in the most exact calculation of effective resonance cross sections could not be solved. Such a calculation should be based on the multilevel formula for cross sections in an infinite dilution. The final composition and the geometrical fine structure should be considered from the beginning of the calculation of screened cross sections. Our approach uses the single-level resonance formula. The influence of the variation in collision density due to a resonance,  $k$ , on the effective cross section of another resonance,  $\ell$ , is not considered. Hwang, [18], has shown that this effect is of the same order as the partial interaction effect we have considered in Dorix. In the calculation of this effect several rather coarse approximations have been made, but this is motivated by the fact that the effect is small. Further, the accuracy of the "intermediate resonance approximation", [5], is not investigated for the case when

the interference between potential and resonance scattering is considered. It is derived for a single resonance together with smooth cross sections of scattering elements. Also, under these conditions the accuracy of only the resonance integral is optimised, but not the accuracy of the screened cross section. Finally, the Dorix programme considers heterogeneity effects in a very approximate way. A comparison between this method and a more accurate one which calculates collision probabilities point-by-point over the resonances is made by Hummel, [11]. The results indicate that the calculated cross sections using the equivalence principle are too small. They are of course strongly dependent upon how the quantity  $a$  in Eq. (4.2) is chosen.

The advantages with the present system are:

- a) a calculation of screened cross sections in Dorix is comparatively fast and can easily be made for a variety of resonance parameter sets for each of the important isotopes. This is especially worth while as long as the parameters are not very well known.
- b) the energy points and groups for which the cross sections are tabulated in the Speng library are quite arbitrary. Thus, a given energy region may contain screened cross sections for fuel isotopes, densely tabulated point-by-point cross sections for some structural elements with resonances in that region and slowly varying cross sections with widely spaced energy points for other elements. This makes the library relatively compact and easily reviewed.
- c) the calculations of neutron spectrum and macroscopic cross sections are so fast that they can be made as routine operations in system studies. The choice of group structure is then quite arbitrary and can be accommodated to the subsequent type of calculation.

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## APPENDIX A

### CALCULATION OF THE INTERACTION EFFECT BETWEEN CORRELATED RESONANCES IN THE UNRESOLVED REGION

We assume that there are no uncorrelated resonances present in the given energy group. With a peak resonance cross section,  $\sigma_{o,k}$ , given by Eq. (2.9) and defining  $\beta_k$  by Eq. (2.23), where  $\lambda_k = 1$ , we obtain the following expression for the resonance integral in group  $g$ :

$$RI_{x,g}^{(i)} = \frac{\sigma_{p,i}^{eff}}{E_g} \sum_k \frac{\Gamma_{x,k}}{\Gamma_k} \int_{\Delta E} \frac{\psi_k dE}{\psi_k + \beta_k \sum_{l \neq k} \frac{\sigma_{o,l}}{\sigma_{o,k}} \psi_l} \quad (A.1)$$

Following Froelich, [10], we develop the inverse of the denominator of the integrand in a Taylor series and preserve the two first terms only. We then obtain:

$$RI_{x,g}^{(i)} \approx \frac{\sigma_{p,i}^{eff}}{E_g} \sum_k \frac{\Gamma_{x,k}}{\Gamma_k} \left\{ J(\theta_k, \beta_k) - \sum_{l \neq k} \frac{\sigma_{o,l}}{\sigma_{o,k}} \int_{\Delta E} \frac{\psi_k \psi_l dE}{(\psi_k + \beta_k)^2} \right\} \quad (A.2)$$

For the  $\psi$ -function we assume the asymptotic (Gaussian) approximation:

$$\psi(E_k - E) = \frac{\sqrt{\pi}}{2} \theta_k e^{-\left[ \frac{\theta_k(E_k - E)}{\Gamma_k} \right]^2} \quad (A.3)$$

This approximation is acceptable in the higher energy range. Its application may be doubtful in the lower end of the unresolved resonance region for fissile isotopes. Experience has shown that there is an abrupt decrease in the interaction effect for these isotopes when the calculational methods change going from the resolved to the unresolved region.

In the second term on the r. h. s. of Eq. (A.2), the denominator of the integrand is assumed to be constant. The integral can then be solved analytically. Further, the summation over the  $l$ -resonances is made by introducing the corresponding probability function. We define

$\Omega(D)dD$  as the frequency with which resonances occur at the distance  $D$  from a given resonance and within the interval  $dD$ . Assuming that the probability function for the distance  $D$  between two resonances is a  $\chi^2$ -distribution with 10 degrees of freedom, Froelich has derived the following expression for  $\Omega$ :

$$\Omega(x) = \sum_{K=1}^5 \cos\left(\frac{2\pi K}{5} + 5x \cdot \sin\frac{2\pi K}{5}\right) \exp\left[5x \cdot \left(\cos\frac{2\pi K}{5} - 1\right)\right] \quad (\text{A. 4})$$

where

$$x = \left(\frac{D}{\bar{D}}\right)$$

Summing over the  $k$ -resonances we obtain average values by introducing the functions  $S_x^{(s)}$ , defined by Eq. (3.5). The final expression for the resonance integral is then:

$$RI_{x, g}^{(i)} \approx \frac{\sigma_{p, i}^{eff}}{E_g} \left[ \frac{\langle \Gamma_x^{(s)} J_x \rangle}{\bar{D}_s} - \frac{\theta_s \bar{D}_s}{\bar{\Gamma}^{(s)} \sqrt{2\pi}} \frac{\langle \sigma_c^{(s)} \rangle \langle \sigma_x^{(s)} \rangle}{\langle \sigma_T^{(i)} \rangle^2} \epsilon\left(\frac{\theta_s \bar{D}_s}{\bar{\Gamma}^{(s)}}\right) \right] \quad (\text{A. 5})$$

where

$$\langle \sigma_c^{(s)} \rangle = 2\pi^2 \frac{\lambda_g^2 g^{(s)}}{\bar{D}_s} \bar{\Gamma}_n^{(s)} \cos 2\delta_{i, l} \quad (\text{A. 6})$$

$$\langle \sigma_x^{(s)} \rangle = \frac{\Gamma_x^{(s)}}{\bar{\Gamma}^{(s)}} S_x^{(s)} \langle \sigma_d^{(s)} \rangle \quad (\text{A. 7})$$

$$\langle \sigma_T^{(i)} \rangle = \langle \sigma_c^{(s)} \rangle + \sigma_{p, i}$$

and

$$\epsilon(z) = 2 \int_0^{\infty} \Omega(x) e^{-\frac{1}{2}(zx)^2} dx \quad (\text{A. 9})$$

$\theta_s$  is obtained by using average resonance parameters. We have here assumed only one resonance series,  $s$ , and this index is therefore equivalent to the isotope index,  $i$ .

The interaction part of the resonance integral is the second term in Eq. (A. 5). The corresponding term in the average flux is obtained in the same way. The expression for the screened cross section when only one resonance series is present is then:

$$\langle \sigma_{x,g}^{(i)} \rangle_{\text{Single } s} = \sigma_{p,i}^{\text{eff}} \frac{\frac{\langle \Gamma_x^{(s)} \rangle_J}{\bar{D}_s} - \frac{\theta \bar{D}_s}{\bar{\Gamma}(s)\sqrt{2\pi}} \frac{\langle \sigma_c^{(s)} \rangle \langle \sigma_x^{(s)} \rangle}{\langle \sigma_T^{(i)} \rangle^2} \epsilon\left(\frac{\theta \bar{D}_s}{\bar{\Gamma}(s)}\right)}{1 - \frac{\langle \Gamma_x^{(s)} \rangle_J}{\bar{D}_s} + \frac{\theta \bar{D}_s}{\bar{\Gamma}(s)\sqrt{2\pi}} \left[ \frac{\langle \sigma_c^{(s)} \rangle}{\langle \sigma_T^{(i)} \rangle} \right]^2} \epsilon\left(\frac{\theta \bar{D}_s}{\bar{\Gamma}(s)}\right) \quad (\text{A. 10})$$

Comparison of Eq. (A. 10) with Eq. (2. 35) gives the following expressions for the interaction effect between correlated resonances:

$$\langle \sigma_{x,i,s,\text{corr}}^{(i)} \rangle = \frac{\sigma_{p,i}^{\text{eff}} \theta \bar{D}_s}{\bar{\Gamma}(s)\sqrt{2\pi}} \frac{\langle \sigma_c^{(s)} \rangle \langle \sigma_x^{(s)} \rangle}{\langle \sigma_T^{(i)} \rangle^2} \epsilon\left(\frac{\theta \bar{D}_s}{\bar{\Gamma}(s)}\right) \quad (\text{A. 11})$$

$$\langle a_{i,s} \rangle = \frac{\theta \bar{D}_s}{\bar{\Gamma}(s)\sqrt{2\pi}} \left[ \frac{\langle \sigma_c^{(s)} \rangle^2}{\langle \sigma_T^{(i)} \rangle} \right] \epsilon\left(\frac{\theta \bar{D}_s}{\bar{\Gamma}(s)}\right) \quad (\text{A. 12})$$

The function  $\epsilon(z)$ , given by Eq. (A. 9) may of course be calculated using an arbitrary level spacing distribution, for example, the Wigner distribution, [18]. But the improvement is not necessarily significant compared to the inaccuracy obtained by using the asymptotic approximation to the  $\psi$ -function.

## APPENDIX B

### CALCULATION OF THE INTERACTION EFFECT BETWEEN UNCORRELATED RESONANCES IN THE UNRESOLVED REGION

Firstly, we assume that only one isotope is present. The screened cross section is then obtained from Eq. (2. 35). The interaction between non-correlated resonances (different series) is given by quantities of the form  $\langle \Gamma J \rangle / \bar{D}$  and  $\langle \Gamma J^* \rangle / \bar{D}$ . In the present case, these quantities may be calculated from rather crude approximations. For each resonance series,  $s$ , we define:



$$h_s = \frac{\langle \Gamma^{(s)} J_s \rangle}{\bar{D}_s} \quad (\text{B.1})$$

This quantity is calculated with good accuracy in Dorix. It is identical with the definition in Eq. (2.37) if the isotope has only one resonance series. We define the quantity  $h_s^*$  in an equivalent way, by changing the indices  $i$  to indices corresponding to the series  $s$ . The function  $J^*$  is defined by Eq. (2.33).

Further, we define a quantity  $h_{s,\infty}$  by the following expression:

$$h_{s,\infty} = \frac{\pi}{2} \frac{\langle \Gamma^{(s)} \sigma_o^{(s)} \rangle}{\bar{D}_s \sigma_{p,i}^{\text{eff}}} \quad (\text{B.2})$$

where  $\sigma_o^{(s)}$  is a resonance peak cross section in series  $s$ .  $h_{s,\infty}$  corresponds to  $h_s$  for infinite dilution.

Now we shall express the quantity  $h_s^*$  as a function of  $h_s$  and  $h_{s,\infty}$ . This is possible if we make the following assumptions:

- a) the resonance parameters are all equal to their average values.
- b) the interdependence between  $J$  and  $J^*$  is independent of the temperature. In this case, a formula can be derived from the assumption that  $T = 0$  and applied to the general case. This assumption is of course quite arbitrary and must be checked against more exact calculations.

For  $T = 0$ , the expression for the  $J$ -function is

$$J_s = \frac{\pi}{2\sqrt{\beta_s(1+\beta_s)}} \quad (\text{B.3})$$

Thus,

$$\beta_s \frac{dJ_s}{d\beta_s} = -\frac{1}{2} \frac{1+2\beta_s}{1+\beta_s} J_s \quad (\text{B.4})$$

We assume that  $\beta_s$  is constant for series  $s$ . The assumption a) and b) also give:

$$h_s = \frac{\pi \Gamma(s)}{2 \bar{D}_s \sqrt{\beta_s (1 + \beta_s)}} \quad (\text{B. 5})$$

and

$$h_{s, \infty} = \frac{\pi \Gamma(s)}{2 \bar{D}_s \beta_s} \quad (\text{B. 6})$$

From Eq:s (B. 5) and (B. 6) we obtain:

$$\beta_s = \frac{1}{\left(\frac{h_s}{h_{s, \infty}}\right)^2} - 1 \quad (\text{B. 7})$$

Eq:s (B. 4), (B. 7), and (2. 33) give finally, after some algebra,

$$J_s^* = \frac{1}{2} J_s \left[ 1 - \left(\frac{h_s}{h_{s, \infty}}\right)^2 \right] \quad (\text{B. 8})$$

Eq. (B. 8) is exact for  $T = 0$  under the assumption a), but can formally be applied to all temperatures. An investigation of its accuracy by a comparison to more accurate numerical calculations is made in Ref. [17].

The corresponding expression for  $h_s^*$  is obtained by making use of assumption a) once again:

$$h_s^* = \frac{1}{2} h_s \left[ 1 - \left(\frac{h_s}{h_{s, \infty}}\right)^2 \right] \quad (\text{B. 9})$$

The interaction between non-correlated resonances is given by Eq. (2. 32) for the resonance integral and by the last part of the r. h. s. of Eq. (2. 34) for the average flux. In the calculation of the screened cross section, some of the terms cancel. The remaining terms can be found from Eq. (2. 35). If the interaction part of the numerator is  $G_{1, s}$ , we have

$$G_{1, s} = h_s^* \sum_{t \neq s} (h_t - h_t^*) \quad (\text{B. 10})$$

The corresponding part of the denominator is:

$$G_{2,s} = \sum_{p \neq s} h_p \sum_{q \neq p} (h_q - h_q^*) - h_s \sum_{t \neq s} h_t^* \quad (\text{B.11})$$

For the calculation of the interaction effect between different resonance series in the same isotope we then use Eq:s (B.10) and (B.11) together with (B.1), (B.2), and (B.9). For the interaction between different isotopes, these quantities are not available. We then introduce the quantities  $h_i$  and  $h_i^*$ , defined by Eq:s (2.37) and (2.38). Neglecting the interaction terms in Eq. (2.35) and assuming that only one resonance series gives a significant contribution to the cross section we obtain the approximate expression:

$$h_i = \frac{\langle \sigma_{r,g}^{(i)} \rangle}{\sigma_{p,i}^{\text{eff}} + \langle \sigma_{r,g}^{(i)} \rangle} \quad (\text{B.12})$$

where  $\langle \sigma_{r,g}^{(i)} \rangle$  is the average total resonance cross section. If we now apply the assumptions a) and b) to all resonances within an isotope,  $h_i^*$  is obtained from Eq. (B.9) by changing the index  $s$  to the isotope index  $i$ . If corresponding changes are made in Eq:s (B.10) and (B.11), these equations give the interaction effect between different isotopes and may be inserted into Eq. (2.36) to give the final screened cross sections. But in the Speng programme this is not possible because we don't know the zero order terms in Eq. (2.36) with sufficient accuracy. But, using instead Eq. (2.41), the zero order term is  $\langle \sigma_{x,g} \rangle$  which is obtained by interpolation in the library. The interaction effect is then given by the remaining factor. This contains only quantities of the types  $h_i$  and  $h_i^*$  which are obtained in the way we have described.





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