

Resonance Models Summary

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1 Introduction

The purpose of this analysis is to formulate means to account for “self-shielding.” Let $\phi(E)$ denote the true flux density in energy, denoted “flux” from here. Self-shielding is the phenomenon of flux drop at resonant energies. It is prohibitively expensive to discretize in energy sufficiently to explicitly model the flux behavior: such calculations are occasionally done (called “ultrafine group calculations”), but cannot be repeatedly done in practical analysis. Resonance models are used as an approximate way to deal with the problem. The idea is to make some assumptions about the behavior of the flux at or near the resonance, to then modify the resonant cross section (“account for self-shielding,” or simply “self-shield”), such that a coarse flux calculation produces an approximately accurate reaction rate, when the flux and self shielded cross section product is integrated over the now smooth cross section.

This paper presents flux factorization, and how it leads to the Narrow, Wide and Intermediate Resonance models. It generally follows sections 8.1 and 8.2 in Reuss’ *Neutron Physics*, section 4.2.3 in Hébert’s *Applied Reactor Physics*, section 8.II.C in Duderstadt and Hamilton’s *Nuclear Reactor Analysis* and sections 3.4 and 5.4 in Henry’s *Nuclear-Reactor Analysis*.¹ Other chapters from these books are also utilized at various points.

2 Approximate Macroscopic Flux Derivation

We make several assumptions to analyze spectrum for resonant (“intermediate”) energies. Consider the following assumptions:

Assumption 1. The reactor is infinite, steady-state and homogeneous.

Assumption 2. No neutrons are born at the energies of interest.

Assumption 3. All scattering events are elastic and isotropic in CMCS.

We first want to estimate its asymptotic behavior— that is, how $\phi(E)$ behaves far from resonances, or in their absence. In this paper, all cross sections and other properties are composition-wide (i.e., total cross section Σ_t), unless indicated otherwise (i.e., total cross

¹This is a different book from Duderstadt and Hamilton’s more popular *Nuclear Reactor Analysis*.

section Σ_t^j of isotope j). For the derivation of the estimate of the macroscopic flux, we only consider energies at which the flux does behave asymptotically; such energies are sufficiently far from isolated resonances.

Let this approximate asymptotic (or “macroscopic”) flux be denoted $\tilde{\psi}(E)$. Note, that the true asymptotic flux will be formulated later, during factorization; this following derivation is only a simplification, to get an idea about the energy dependence of $\tilde{\psi}(E)$. Let the slowing-down density (also known as the “slowing-down current”) at the bottom of source energies (that is, with all of the sources and source energy absorptions accounted for) be denoted q_s ; this quantity has units of neutrons/cm³s, and corresponds to the rate density (in space) of neutrons slowing down past energy E_s , which is the bottom of the source energies. Next, consider an energy E_0 , well above an isolated resonance of interest, and well below the next resonance, near which we want to compute the macroscopic flux. Recognizing that neutrons slowing down past E_s can only be absorbed or keep slowing down, we can evaluate the slowing-down density q_0 as:

$$q_0 = q_s - \int_{E_0}^{E_s} dE' \Sigma_a(E') \phi(E'). \quad (1)$$

While the integral in Eq. (1) is obviously difficult to evaluate, it is still a constant for a given E_0 .

To evaluate the asymptotic behavior of the flux outside resonances, one additional assumption is necessary:

Assumption 4. There is no absorption at energies where flux behaves asymptotically.

Note, that assumption 4 does not invalidate Eq. (1), because the integral in Eq. (1) accounts for in-resonance absorptions as well.

Let ξ_j denote the average lethargy gain from collision with isotope j . Under assumption 3, it is given by:

$$\xi_j = 1 - \frac{(A_j - 1)^2}{2A_j} \ln \left(\frac{A_j + 1}{A_j - 1} \right), \quad (2)$$

in which A_j is the mass number of isotope j .

With several scattering isotopes, a composition-average lethargy gain per collision $\bar{\xi}(E)$ can be formulated:

$$\bar{\xi}(E) = \frac{\sum_{\text{all } j} \xi_j \Sigma_s^j(E)}{\sum_{\text{all } j} \Sigma_s^j(E)} = \frac{\sum_{\text{all } j} \xi_j \Sigma_s^j(E)}{\Sigma_s(E)}. \quad (3)$$

Denoting the isotope j energy differential scattering cross section $\Sigma_s^j(E' \rightarrow E)$, we can utilize assumption 3 to express it as:

$$\Sigma_s^j(E' \rightarrow E) = \begin{cases} \Sigma_s^j(E') \frac{1}{E' (1 - \alpha_j)} & \text{if } \alpha_j E' \leq E \leq E' \\ 0 & \text{otherwise.} \end{cases} \quad (4)$$

in which α_j is the reduced mass of isotope j , given by:

$$\alpha_j = \left(\frac{A_j - 1}{A_j + 1} \right)^2. \quad (5)$$

Equation (2) can be rewritten in terms of α_j :

$$\xi_j = 1 + \frac{\alpha_j}{1 - \alpha_j} \ln(\alpha_j). \quad (6)$$

Assumption 4 requires the slowing-down density $q(E)$ at all energies $E < E_0$ (above an isolated resonance of interest) to be equal to q_0 , to conserve neutrons. Using the differential scattering cross section from Eq. (4), and using $\tilde{\psi}(E)$ as the flux at the energies of interest, we can express $q(E)$:

$$q(E) = q_0 = \sum_{\text{all } j} \left[\int_E^{E/\alpha_j} dE' \int_{\alpha_j E'}^E dE'' \frac{\Sigma_s^j(E') \tilde{\psi}(E')}{E' (1 - \alpha_j)} \right]. \quad (7)$$

In Eq. (7), energies E' and E'' represent all potential initial energies for scatter through E , and all potential target energies for scatter through E , respectively.

Equation (7) can be solved to yield $\tilde{\psi}(E)$. It is not, however, analytically solvable, because of the (so far) arbitrary energy dependence of $\Sigma_s^j(E)$. Because the energies of interest are in the intermediate range, and far from resonances (hence macroscopic flux is applicable), we can make an additional assumption:

Assumption 5. At energies where the flux behaves asymptotically, the scattering cross sections of all isotopes have the same shape in energy.

Assumption 5 can be expressed as follows:

$$\Sigma_s^j(E) = \bar{\Sigma}_s^j \zeta(E) \quad \forall j, \quad (8)$$

in which $\bar{\Sigma}_s^j$ is the averaged (over an energy interval of interest, like an energy group) scattering cross section of isotope j , and $\zeta(E)$ is the energy shape function for all scattering cross sections.

Equation (8) significantly simplifies Eq. (3), turning $\bar{\xi}$ into a constant:

$$\bar{\xi} = \frac{\sum_{\text{all } j} \xi_j \bar{\Sigma}_s^j}{\sum_{\text{all } j} \bar{\Sigma}_s^j} = \frac{\sum_{\text{all } j} \xi_j \bar{\Sigma}_s^j}{\bar{\Sigma}_s}. \quad (9)$$

Equation (7) is similarly simplified:

$$q_0 = \sum_{\text{all } j} \left[\frac{\bar{\Sigma}_s^j}{1 - \alpha_j} \int_E^{E/\alpha_j} dE' \int_{\alpha_j E'}^E dE'' \frac{\zeta(E') \tilde{\psi}(E')}{E'} \right]. \quad (10)$$

Equation (10) is now solvable analytically, and yields:

$$\tilde{\psi}(E) = \frac{q_0}{E \bar{\xi} \bar{\Sigma}_s \zeta(E)}. \quad (11)$$

Assumptions 1–5 are all required to yield Eq. (11).

Nonresonant materials (moderators, other light isotopes and heavy isotopes with self-shielding accounted for) generally have a nearly constant scattering cross section at the energies of interest, because they are either light or self-shielded, and so do not exhibit resonant behavior. Resonant (heavy) isotopes, however, obviously do. Inelastic scattering is not present at the intermediate energies, but elastic scattering for resonant isotopes actually consists of two different reaction types: potential scattering and resonant elastic scattering. (Inelastic scattering is another form of resonant scattering, occurring at high energies.) Furthermore, resonant elastic scattering consists of two mathematically different phenomena: the resonance itself, and the “interference” (between resonance and potential scattering) term. An inspection of the Single-Level Breit-Wigner equation for $s = 0$ elastic scattering shows each term. Note, that while the interference term is commonly neglected, it is actually the term responsible for the drop in elastic scattering cross section below each resonance (the term varies as $(E - E_{res})$, and so is negative under the resonance). This phenomenon is most noticeable on Iron-56.

Potential scattering cross section is very nearly a constant over intermediate energies (not truly constant — the billiard ball collision model is only an approximation), but resonant elastic scattering is not: it follows the same resonant behavior as resonant capture cross section. In this analysis, and almost always in self-shielding calculations, the resonant and interference terms are treated together, and the potential scattering is assumed constant.

We can combine the two to yield the full elastic scattering cross section:

$$\Sigma_s^*(E) = \Sigma_p^* + \Sigma_r^*(E), \quad (12)$$

in which the subscripts s , p and r indicate the full, potential and resonant elastic scattering, respectively.² The superscripts $*$ and $+$ indicate the single resonant and all nonresonant isotopes together, respectively.

Outside of resonances, the nonresonant isotopes’ scattering cross section is nearly constant. The only scattering cross section that a resonant isotope has outside of resonances is the potential scattering cross section, which is also a constant. This justifies another assumption, which replaces assumption 5:

Assumption 6. At energies where the flux behaves asymptotically, all scattering cross sections are constant.

This assumption can be expressed as:

$$\zeta(E) = 1, \quad (13)$$

which further simplifies Eq. (11):

$$\tilde{\psi}(E) = \frac{q_0}{E\bar{\xi}\bar{\Sigma}_s}. \quad (14)$$

The key result in the above derivation is that $\tilde{\psi}(E)$ is linearly proportional to $1/E$. We can now address resonances.

² σ_p is also sometimes used to denote the (n,p) cross section, a subset of capture.

3 Flux Factorization

To consider the flux within the resonance, we factor the full flux $\phi(E)$ into a macroscopic flux $\psi(E)$ and a fine structure function (also known as the “fine structure factor”, or “self-shielding factor”) $\varphi(E)$, as follows:

$$\phi(E) = \psi(E) \varphi(E). \quad (15)$$

Note, that this macroscopic flux $\psi(E)$ is different from $\tilde{\psi}(E)$; they both have the $1/E$ dependence (discussed below), but $\psi(E)$ is not necessarily given by either Eq. (11) or (14).

By nature of nonresonant isotopes, another assumption is made, similar to assumption 6:

Assumption 7. All nonresonant isotopes’ cross sections are constant.

Let us denote the nonresonant and resonant slowing-down operators \hat{R}^+ and \hat{R}^* , respectively. Let all nonresonant isotopes be indexed by j^+ . Considering assumption 7, the operators are then given by:

$$\hat{R}^+ \phi(E) = \sum_{\text{all } j^+} \left[\int_E^{E/\alpha_{j^+}} dE' \frac{\Sigma_s^{j^+}}{E' (1 - \alpha_{j^+})} \phi(E') \right], \quad (16a)$$

$$\hat{R}^* \phi(E) = \int_E^{E/\alpha^*} dE' \frac{\Sigma_s^*(E')}{E' (1 - \alpha^*)} \phi(E'). \quad (16b)$$

The slowing-down equation models $\phi(E)$ both at and outside of resonances, with only assumptions 1 – 3 and 7. It is given by:

$$[\Sigma_t^+ + \Sigma_t^*(E)] \phi(E) = \hat{R}^+ \phi(E) + \hat{R}^* \phi(E). \quad (17)$$

To resolve the flux behavior at and outside of resonances, we substitute Eq. (15) into Eq. (17):

$$[\Sigma_t^+ + \Sigma_t^*(E)] \psi(E) \varphi(E) = \hat{R}^+ \psi(E) \varphi(E) + \hat{R}^* \psi(E) \varphi(E). \quad (18)$$

Next, we define $\psi(E)$ in terms of $\phi(E)$ to yield:

$$\psi(E) = \frac{1}{\Sigma_s^+} \hat{R}^+ \phi(E). \quad (19)$$

This definition serves two purposes. First, it is a generalization of Eq. (14), with assumptions 4 and 6 lifted and replaced by the much less restrictive assumption 7. With assumptions 4 and 6, it can be shown that Eq. (19) reduces to Eq. (14). Second, writing the macroscopic flux in this form simplifies the nonresonant slowdown term in Eq. (18):

$$[\Sigma_t^+ + \Sigma_t^*(E)] \psi(E) \varphi(E) = \Sigma_s^+ \psi(E) + \hat{R}^* \psi(E) \varphi(E). \quad (20)$$

$\psi(E)$ can be thought of as the flux that would be generated if the nonresonant isotopes only moderated, but did not absorb, and there were no resonant isotopes. As such, based on section 2, we can make the following assumption:

Assumption 8. The macroscopic flux shape in energy, within the group of interest, is $1/E$.

Under assumption 8, the macroscopic flux $\psi(E)$ can be written as follows:

$$\psi(E) = C_g \frac{1}{E}, \quad (21)$$

in which C_g is a scaling constant of the macroscopic flux in the energy group of interest. Because of its $1/E$ shape, $\psi(E)$ is a constant in lethargy. $\psi(E)$ has units of neutrons/cm²s eV, so $\varphi(E)$ is dimensionless. The full flux is now factored further:

$$\phi(E) = C_g \frac{1}{E} \varphi(E). \quad (22)$$

The $1/E$ dependence of $\psi(E)$ is not explicitly seen when treating this problem in terms of lethargy. It arises implicitly in the assumption of constant macroscopic flux density in lethargy, which is equivalent to a $1/E$ dependence, as shown later.

Equation (21) simplifies the resonant slowing-down operator:

$$\hat{R}^* \phi(E) = C_g \hat{R}^* \left\{ \frac{\varphi(E)}{E} \right\}. \quad (23)$$

Substituting Eqs. (21) and (23) into Eq. (20) and dividing by C_g yields the slowdown equation for the fine structure factor:

$$[\Sigma_t^+ + \Sigma_t^*(E)] \frac{\varphi(E)}{E} = \frac{\Sigma_s^+}{E} + \hat{R}^* \left\{ \frac{\varphi(E)}{E} \right\}. \quad (24)$$

Equation (24) is frequently written in terms of microscopic cross sections. To rewrite it like that, we define several new quantities. Let \hat{r}^* be the microscopic version of the resonant slowdown operator, given by:

$$\hat{r}^* \left\{ \frac{\varphi(E)}{E} \right\} = \frac{1}{N^*} \hat{R}^* \left\{ \frac{\varphi(E)}{E} \right\} = \frac{1}{1 - \alpha^*} \int_E^{E/\alpha^*} dE' \frac{\sigma_s^*(E')}{(E')^2} \varphi(E'), \quad (25)$$

in which N^* is the atom density of the resonant isotope.

Let σ_d be the “dilution cross section,” which can be thought of as the number of barns of nonresonant materials per atom of resonant material, given by:

$$\sigma_d = \frac{\Sigma_t^+}{N^*}, \quad (26)$$

and the *gamma factor* γ to be given by:

$$\gamma = \frac{\Sigma_s^+}{\Sigma_t^+}. \quad (27)$$

The purpose of both quantities is to be used in the microscopic version of the slowdown equation, as follows:

$$[\sigma_d + \sigma_t^*(E)] \frac{\varphi(E)}{E} = \gamma \frac{\sigma_d}{E} + \hat{r}^* \left\{ \frac{\varphi(E)}{E} \right\}. \quad (28)$$

It is important to note that through Eq. (28), the fine structure factor $\varphi(E)$ accounts not only for the resonance itself, but also for the nonresonant absorption (through γ), and for any other cross section variation of the resonant isotope in over the energies of interest.

In a nonresonant composition, the fine structure factor reduces to γ :

$$\varphi_{\infty}(E) = \gamma. \quad (29)$$

This makes sense: the macroscopic flux accounts for all nonresonant physics except absorption, which γ factor models. This is not an exact model, but it is an unavoidable approximation made by separating the two flux components.

The primary purpose of finding $\varphi(E)$ is to construct a self-shielded cross section (a group cross section), which can then be used by a macroscopic flux calculator to solve for C_g . Together, the macroscopic flux and the self-shielded cross sections provide all groupwise reaction rates required for reactor analysis, so once the group cross sections have been constructed, the fine structure factors have no further use.

To evaluate the resonant isotope's group cross section of reaction type T in energy group g bounded by $E \in [E_g, E_{g-1}]$ based on a known fine structure factor, with all of the above assumptions that went into the formulation of $\varphi(E)$, we take the flux shape product $\varphi(E)/E$, and use it to weight the cross section through the following calculation:

$$\bar{\sigma}_{T,g}^* = \frac{\int_{E_g}^{E_{g-1}} dE \frac{1}{E} \sigma_T^*(E) \varphi(E)}{\int_{E_g}^{E_{g-1}} dE \frac{1}{E} \varphi(E)}. \quad (30)$$

Some self-shielded data is provided with ENDF-B/VII.1, as “averaged cross section” under the Covariances Data (BOXER) tape. These are only examples for some specific dilutions, and cannot be used for true calculations, but they do illustrate what self-shielded cross section data looks like.

Equation (30) is equivalent to weighting the cross section through the full flux $\phi(E)$, with the macroscopic flux constant C_g cancelling out. Only the flux shape in energy matters for Eq. (30). The same is true for any constant scaling coefficients of the fine structure factor, such as γ .

The integrals in Eq. (30) are also frequently taken in lethargy u :

$$u = \ln\left(\frac{E_{max}}{E}\right), \quad (31)$$

in which E_{max} is some constant reference energy, usually the maximum energy a neutron can have in the reactor; for the purposes of analyzing an energy group $E \in [E_g, E_{g-1}]$, we can set $E_{max} = E_{g-1}$. Because $\varphi(E)$ and $\sigma_T^*(E)$ are not densities in energy or in lethargy, they can easily be converted to lethargy using Eq. (31).

To convert an integral in energy into an integral in lethargy, we need to convert the the integrand and the differential from being energy-dependent to lethargy-dependent, and

to convert the group boundaries to being lethargy values. $\varphi(E)$ and $\sigma_T^*(E)$ are converted trivially, as discussed above. The group boundaries E_g and E_{g-1} can be converted into lethargies through Eq. (31). To convert the differential, we need to relate dE and du , by differentiating and rearranging Eq. (31), as follows:

$$du = -\frac{1}{E}dE, \quad (32)$$

which indicates that a $1/E$ shape in energy is a constant in lethargy. This is applicable to the macroscopic flux, which, being a $1/E$ dependence, is represented as a constant in lethargy, which can simplify a lot of the analysis in this section.

Substituting all of these conversions into Eq. (30) yields:

$$\bar{\sigma}_{T,g}^* = \frac{\int_{u_{g-1}}^{u_g} du \sigma_T^*(u) \varphi(u)}{\int_{u_{g-1}}^{u_g} du \varphi(u)}, \quad (33)$$

in which both integrals have been flipped, because of the minus sign in Eq. (32).

Note, that although there is now no explicit mention of the macroscopic flux in Eq. (33), its $1/E$ shape in energy (constant in lethargy) effect on the integrals was not dropped — rather, it became incorporated in the differentials, through Eq. (32). Therefore, Eqs. (30) and (33) are completely equivalent, and yield the same answer for the same fine structure factor and cross section.

Besides being used for group cross section generation, $\varphi(E)$ can also be used to reconstruct the full flux $\phi(E)$ for various purposes, using Eqs. (22). Doing so requires a group flux Φ_g , which is the integral of the full flux over group g ; the group fluxes are computed through various multigroup calculations, both homogeneous and heterogeneous. The combined energy dependence of $\psi(E)$ and $\varphi(E)$, which is $\varphi(E)/E$, is then used as the shape function of the reconstructed full flux in group g , as follows:

$$\Phi_g = C_g \int_{E_g}^{E_{g-1}} dE \frac{\varphi(E)}{E}. \quad (34)$$

This full flux reconstruction is generally avoided in favor of simply computing the group fluxes Φ_g , because those, together with group cross sections, yield the group reaction rates.

To find $\varphi(E)$, it is now necessary to somehow approximate $\hat{r}^* \left\{ \varphi(E)/E \right\}$. It can be done by solving Eq. (28) directly, or by estimating it through a resonance model. The direct solution is briefly discussed in section 4, and the resonance models in the following sections.

4 Fine Structure Factor Calculation

An inspection of a heavy isotope like Uranium-238 shows that it has about a thousand resolved resonances. Resolving them directly would require over ten thousand energy groups,

which is prohibitively expensive to use in every self-shielding calculation. For this reason, multiple resonances are usually put into a single group. To calculate the fine structure factor in this group, the following equation is then solved by a self-shielding code (or, more frequently, a self-shielding module of a code):

$$\left[\sigma_d + \sigma_t^*(E) \right] \frac{\tilde{\varphi}(E)}{E} = \frac{\sigma_d}{E} + \hat{r}^* \left\{ \frac{\tilde{\varphi}(E)}{E} \right\}. \quad (35)$$

$\tilde{\varphi}(E)$ in Eq. (35) is very similar to $\varphi(E)$, but does not account for absorption by nonresonant isotopes. It can be accounted for through γ :

$$\varphi(E) = \gamma \tilde{\varphi}(E). \quad (36)$$

It is important to note, that while the scale of $\varphi(E)$ does not matter in the treatment presented in this paper (as all nonresonant properties are constant), in some more advanced self-shielding techniques assumption 7 is modified, so it is a good practice to correctly retain the scale of $\varphi(E)$ even in simple cases.

As shown in Eq. (30), $\varphi(E)$ can be used to calculate all self-shielded cross sections of the resonant isotope. Because $\hat{r}^* \tilde{\varphi}(E)$ is normally a function of the flux in the group above, either assumptions have to be made about this behavior, or Eq. (35) needs to be solved for multiple energy groups at once (in which case the nonresonant parameters can no longer be considered constant). A true solution of Eq. (35) is generally expensive, because it requires an ultrafine group discretization (multiple energy groups within each resonance), so resonance models are frequently used to account for individual resonance, which self-shields the cross-sections across those resonances and simplifies the calculation. Only low energy resonances are usually solved directly through an ultrafine discretization, because models do not represent them sufficiently accurately.

The only property in Eq. (35) that is not specific to the resonant isotope is the dilution cross section σ_d . This allows the self-shielding code to tabulate, in advance, all self-shielded microscopic cross sections of important isotopes as functions of dilution and temperature (resonance parameters depend heavily on temperature). Because a tabulated result is sufficient, it does not need to be repeated, unless the tabulation is insufficient for a given set of temperatures and dilution cross sections; this justifies the occasional use of ultrafine calculations.

Resonance models approximate $\varphi(E)$ over resonances by making simplifying assumptions about the behavior of the flux within and near them. Using a resonance model allows the self-shielding code to avoid the ultrafine discretization within that resonance, and so is desired, if the model is sufficiently accurate. The simplest model, the narrow resonance model, is discussed in the next section.

5 Narrow Resonance Model

The Narrow Resonance (NR) model relies on the following assumptions:

Assumption 9. The resonance is isolated: there is no interference from other resonances.

Assumption 10. The width of the resonance is negligibly small compared to the average energy loss per collision with the resonant isotope.

Assumption 10 implies that a neutron can only scatter into a resonance from an energy higher than within the resonance. At those energies, the resonant isotope's scattering cross section is only the potential cross section σ_p^* and the fine structure factor is $\varphi_\infty(E)$, as per Eq. (29). Substituting these into Eq. (25) yields:

$$\hat{r}^* \left\{ \frac{\varphi(E)}{E} \right\} = \frac{1}{1 - \alpha^*} \int_E^{E/\alpha^*} dE' \frac{\sigma_p^*}{(E')^2} \varphi_\infty(E') = \gamma \frac{\sigma_p^*}{E}. \quad (37)$$

Substituting Eq. (37) and $\varphi_\infty(E)$ into Eq. (28) yields:

$$\left[\sigma_d + \sigma_t^*(E) \right] \frac{\varphi(E)}{E} = \gamma \frac{\sigma_d}{E} + \gamma \frac{\sigma_p^*}{E}, \quad (38)$$

rearranging which yields $\varphi_{NR}(E)$, the fine structure function computed through the Narrow Resonance model:

$$\varphi_{NR}(E) = \gamma \frac{\sigma_d + \sigma_p^*}{\sigma_d + \sigma_t^*(E)}. \quad (39)$$

$\varphi_{NR}(E)$ is also known as the Bondarenko flux.

Because the effective number density associated with the dilution cross section is N^* , that of the resonant isotope, $\varphi_{NR}(E)$ can be modified as follows

$$\varphi_{NR}(E) = \gamma \frac{\Sigma_t^+ + \Sigma_p^*}{\Sigma_t(E)}. \quad (40)$$

$\gamma (\sigma_d + \sigma_p^*)$ is essentially a scaling factor, and so can be dropped (ideally should not be, for good practice) when using $\varphi_{NR}(E)$ in Eq. (30).

The narrow resonance model works best at the top of the resolved resonance range, because assumption 10 is most applicable there. We can note that for an infinite dilution ($\sigma_d \rightarrow \infty$), $\varphi_{NR}(E)$ approaches γ , or $\varphi_\infty(E)$, as it should, by definition of $\varphi_\infty(E)$.

6 Wide Resonance Model

The Wide Resonance (WR) model is sometimes referred to as the Narrow Resonance, Infinite Mass (NRIM) model. It still uses assumption 9, but is based on the opposite assumption from assumption 10:

Assumption 11. The width of the resonance is very large compared to the average energy loss per collision with the resonant isotope.

The “infinite mass” name makes sense: it indicates that the neutron is assumed to lose no energy from a collision with the resonant isotope. This assumption implies that most

neutrons scattering into the resonance scatter from inside the resonance itself; this leads to the product $\sigma_s^*(E) \varphi(E)$ being nearly constant within the resonance. This simplifies Eq. (25):

$$\hat{r}^* \left\{ \frac{\varphi(E)}{E} \right\} = \frac{1}{1 - \alpha^*} \int_E^{E/\alpha^*} dE' \frac{1}{(E')^2} \sigma_s^*(E') \varphi(E') = \frac{\sigma_s^*(E) \varphi(E)}{E}. \quad (41)$$

Substituting Eq. (41) into Eq. (28) yields:

$$\left[\sigma_d + \sigma_t^*(E) \right] \frac{\varphi(E)}{E} = \gamma \frac{\sigma_d}{E} + \frac{\sigma_s^*(E) \varphi(E)}{E}, \quad (42)$$

rearranging which yields $\varphi_{WR}(E)$, the fine structure function computed through the Wide Resonance model:

$$\varphi_{WR}(E) = \gamma \frac{\sigma_d}{\sigma_t^*(E) + \sigma_d - \sigma_s^*(E)}, \quad (43)$$

which can instead be written in terms of $\sigma_a^*(E)$, the resonant isotope's absorption cross section:

$$\varphi_{WR}(E) = \gamma \frac{\sigma_d}{\sigma_a^*(E) + \sigma_d}. \quad (44)$$

As with the narrow resonance model, $\gamma \sigma_d$ is a scaling factor here, and can (but should not) be ignored when building the group cross sections.

The wide resonance model works best near the bottom of the resolved resonance range, because assumption 11 is most applicable there. It is, however, generally less applicable than the narrow resonance model for higher energies of the resolved resonance range.

As for the narrow resonance model, $\varphi_{WR}(E)$ approaches $\varphi_\infty(E)$ with infinite dilution, as it should.

Most resonances of Uranium-238, and many other heavy isotopes, are neither wide nor narrow, and are intermediate in this respect. The intermediate resonance model exists for such resonances.

7 Intermediate Resonance Model

The Intermediate Resonance Model (IR) is also known as the Goldstein-Cohen (GC) approximation. It consists of treating the resonant slowdown operator as a linear combination of of the wide and narrow resonance models, as follows:

$$\hat{r}^* \left\{ \frac{\varphi(E)}{E} \right\} = \lambda_g \frac{\gamma \sigma_p^*}{E} + (1 - \lambda_g) \frac{\sigma_s^*(E) \varphi(E)}{E}, \quad (45)$$

in which λ_g is a weighting parameter, known as the Goldstein-Cohen parameter. $\lambda_g = 0$ corresponds to the wide resonance and $\lambda_g = 1$ corresponds to the narrow resonance models, respectively. It is energy group-specific, and is chosen manually, based on experience.

Substituting Eq. (45) into Eq. (28) yields:

$$\left[\sigma_d + \sigma_t^*(E) \right] \frac{\varphi(E)}{E} = \gamma \frac{\sigma_d}{E} + \lambda_g \frac{\gamma \sigma_p^*}{E} + (1 - \lambda_g) \frac{\sigma_s^*(E) \varphi(E)}{E}, \quad (46)$$

rearranging which yields $\varphi_{IR}(E)$, the fine structure function computed through the Intermediate Resonance model:

$$\varphi_{IR}(E) = \gamma \frac{\lambda_g \sigma_p^* + \sigma_d}{\sigma_t^*(E) + \sigma_d - (1 - \lambda_g) \sigma_s^*(E)}. \quad (47)$$

8 Conclusion

Other resonance models, all of which aim to produce the most accurate group cross sections with the least expensive calculations, exist. All analysis in this paper was done for an infinite homogeneous reactor, but in practice some of the terms of the slowdown equation (normally the dilution cross section) can be adjusted to account for heterogeneity. Note, that the self-shielding module, with such treatment, remains an infinite homogeneous solver, such as the one solving Eq. (35). With such adjustment, however, the dilution cross section is no longer a constant, and becomes a function of energy, which is why it is appropriate to keep the constant (in an infinite homogeneous system) terms within $\varphi(E)$.

Some ultrafine self-shielding procedures use a cylindrical 1-dimensional pin cell geometry with reflective boundary condition, attempting to account for the rim effect and the fine spectrum variation radially across the fuel pin. This approach is generally quite costly, because of the number of groups required.

Appropriate use of self-shielding and other approximations allows one to eventually condense the multigroup parameters to a 2-group approximation in most LWRs. Fast reactors are typically condensed down to about 33 groups. All such approximations require one to account for heterogeneity in order to produce an appropriate weighting spectrum.

Monte-Carlo codes, such as MCNP, do not require self-shielding calculations: they operate in continuous energy, and treat self-shielding, as well as all other effects in a reactor, statistically, instead of treating them as deterministic averages. These calculations are sometimes used to compute fine structure functions.

Lastly, because self-shielding is primarily a function of composition, and not of core layout, some lattice analysis is done based on precomputed multigroup parameters (usually several hundred) for reactors of a given type. Such analysis is heavily experience based, and is generally less accurate than using true self-shielded parameters based on appropriate ultrafine group calculations.