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URANIUM SELF-SHIELDING IN FAST REACTOR BLANKETS

by

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ABSTRACT

The effects of heterogeneity on resonance self-shielding are examined with particular emphasis on the blanket region of the fast breeder reactor and on its dominant reaction - capture in U-238. The results, however, apply equally well to scattering resonances, to other isotopes (fertile, fissile and structural species) and to other environments, so long as the underlying assumptions of narrow resonance theory apply.

The heterogeneous resonance integral is first cast into a modified homogeneous form involving the ratio of coolant-to-fuel fluxes. A generalized correlation (useful in its own right in many other applications) is developed for this ratio, using both integral transport and collision probability theory to infer the form of correlation, and then relying upon Monte Carlo calculations to establish absolute values of the correlation coefficients.

It is shown that a simple linear prescription can be developed for the flux ratio as a function of only fuel optical thickness and the fraction of the slowing-down source generated by the coolant. This in turn permitted derivation of a new equivalence theorem relating the heterogeneous self-shielding factor to the homogeneous self shielding factor at a modified value of the background scattering cross section per absorber nucleus. A simple version of this relation is developed and used to show that heterogeneity has a negligible effect on the calculated blanket breeding ratio in fast reactors.

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CHAPTER 1

INTRODUCTION

1.1 Foreword

Considerable attention has been devoted of late to calculations and measurement of the precise breeding ratio which can be achieved in state-of-the-art LMFBR's (T4) (L7). At MIT a major goal of the ERDA-sponsored Blanket Research Project has been the assessment of the blanket contribution to the breeding gain. Previous calculations (by Leung, et.al. (L6) and by others (L8)) have indicated that heterogeneity may play an important role in the blanket neutron balance. Extensive work by ANL on highly heterogeneous plate-configuration fast critical assembly cores supports this concern (D7). Thus the research reported here was initiated with the objective of carrying out a definitive review of the methods used to account for heterogeneity in FBR physics calculations. As will be discussed in the text, it soon became clear that an independent approach to the problem was called for, which has led to the formulation of a new equivalence theorem, and ultimately to the finding that heterogeneity can not play a dominant role in fast reactor core or blanket neutronic calculations. Finally, in the interest of specificity, the text focuses on resonance capture in U238 in an LMFBR blanket environment, because this is the most highly shielded case encountered in practice. The results, however, are equally

applicable to resonance scattering, to other nuclei, and to other FBR environments (e.g. the LMFBR core, GCFR cores and blankets)

1.2 Background

Replacement of regions having internal structure by equivalent homogeneous regions is a familiar and key step in most reactor physics calculations. In the limiting case when the neutron mean free path between interactions is much larger than the mean distance (chord length) through a unit cell (one fuel pin, its clad and associated coolant), the neutron flux will be spatially uniform and simple volume-fraction-weighted homogenization will suffice. Except for the narrow energy bands centered around resolved resonances, this is very nearly the case in all fast reactor media. Even in the cases involving resonances, a homogeneous treatment is frequently adequate so long as the flux dip due to neutron removal (by absorption or down-scattering) at the resonance is accounted for. Thus an understanding of homogeneous or "energy" self-shielding is an appropriate prerequisite for the topic of heterogeneous self-shielding; particularly since the latter is often treated by slight modifications of the prescriptions developed for the homogeneous case.

Homogeneous self-shielding has been examined in detail by several authors whose work should be familiar to the reader, (B2), (G1), (P3), and therefore the topic need not be dealt with in great

detail here. However we should note that Goldstein's treatment, which handles narrow, intermediate and wide resonances, appears particularly well suited to our present interests, and has been adopted in the IDIOT (P1) and MIDI (R1) programs for FBR applications.

Heterogeneous self-shielding has not been as satisfactorily treated. The simplest and most appealing approach, which appears to have rather widespread use in FBR applications, is to employ an equivalence relation, which relates a heterogeneous configuration to an "equivalent" homogeneous one. It is at this point that an apparent inconsistency becomes evident - which motivated the somewhat different approach taken in the present research. The discussion presented by Bondarenko et al (B2), whose f-factor methodology has gained almost universal acceptance for state-of-the-art FBR calculations (L2), can be used to illustrate this difficulty. In brief, heterogeneity is to be accounted for by adding a (positive) increment to σ_0 , the background scattering cross section per resonance absorbing nucleus. Consider, however, the consequences of this act: increasing σ_0 increases the shielding factor, f ; hence the group absorption cross section is also increased. Thus, increasing the degree of heterogeneity will increase resonance absorption and decrease the resonance escape probability -

a result which is counter-intuitive, and incompatible with thermal reactor physics design principles of long standing.

Other difficulties also became apparent in the course of the work, the principal one involving the functional dependence of the heterogeneous increment on σ_0 , which involves the Dancoff-factor correction for the effect of neighboring rods in a lattice. In view of this inability to reconcile past practice, it was considered justified to introduce an entirely new approach to the problem, which is the focus of the present work.

1.3 Outline

The body of the report which follows parallels in its organization the sequence followed in the conduct of the research. In Chapter 2 a review of so-called energy self-shielding in homogeneous media is presented to develop the perspective needed for the introduction of heterogeneity. In Chapter 3 it is shown that heterogeneity can be accounted for by merely increasing the weight (ratio of coolant to fuel fluxes) assigned to scattering-removal events in the coolant region. Transport and collision probability methods are used to infer a simple prescription for the coolant / fuel flux ratio as a function of the optical thickness of fuel and coolant and the fraction of the (slowing-down) neutron source born in the coolant; Monte Carlo calculations are then used to quantify and verify the functional relation. In

Chapter 4 it is shown that a simple linearized version of the flux ratio relation is justified (by comparison with numerical computations), and is necessary if an equivalence theorem relating heterogeneous and homogeneous self-shielding is to be derived.

Finally the "exact" equivalence theorem, and a simple version suitable for hand calculations, are used to show that heterogeneity has a negligible effect on group cross sections (typically $< 1\%$) and hence on blanket breeding ratio. The concluding Chapter, 5, summarizes the work and proposes follow-on research. It is followed by appendices presenting a computer program used in the research and numerical examples.

CHAPTER 2

HOMOGENEOUS SELF-SHIELDING

In this chapter we will review the general topic of self-shielding in homogeneous media, with particular emphasis on fertile nuclei in fast reactors. Several objectives will be kept in mind: relation of the present work to past and current practice in the field, introduction of basic concepts necessary for extension of methodology to heterogeneous media in later chapters, and verification of the numerical accuracy of our calculations in a limiting case (infinitely dilute absorber) for which analytical results are known.

2.1 Energy Self-Shielding

The local neutron flux in a fast reactor varies in both energy (lethargy) and space. In this chapter, concern will be limited to the variation in energy, neglecting both the global and fine-structure variations as a function of spatial position. While

the resultant formulation is strictly applicable only to the infinite homogeneous reactor, it turns out that most of the self-shielding effects in fast reactors are primarily due to this energy-related phenomenon.

If neutrons are supplied at lethargy u by elastic or inelastic downscattering, and removed by absorption or scattering with a large energy loss, the following simple balance applies:

$$\Sigma_R(u)\phi(u)\Delta u = S(u), \quad (2-1)$$

where $\Sigma_R(u)$ is the removal cross section at lethargy u

$\phi(u)$ is the flux per unit lethargy at lethargy u

$S(u)$ is the source slowing down past lethargy u .

Thus if $S(u)$ is a smooth, continuous function of u , $\phi(u)$ will display fine structure inversely related to the fine structure in $\Sigma_R(u)$. The effects of resonance absorption and scattering are especially pertinent here.

Because the flux dips where resonances peak, the reaction rate (product of flux and cross section) is less than that calculated using an unperturbed flux. Since it is most convenient to carry out reactor calculations using neutron groups much wider in lethargy or energy space than resonance-induced fine structure, some sort of averaging process must be applied to both the flux and the cross

section in order to insure that reaction rates are conserved — an essential feature if the neutron balance is to be correctly determined.

In the case of the flux, the dips are usually narrow compared to group width, and it is customary to use the lethargy (energy)-integrated unperturbed flux as the total group flux. Very often standard spectra, such as $\phi(E) \sim 1/E^n$, are assumed for the intra-group shape of the unperturbed flux in energy space. Neglecting resonance-induced flux dips in computing total group flux involves an error in the flux integral less than roughly

$$\frac{\Gamma + \Delta}{D}$$

where Γ is the resonance width, Δ is the doppler width, and D is the spacing between resonances. For U-238, for example, the error would be less than or equal to about 0.4 % (Fig 2.1).

Thus the problem reduces to computation of effective group cross sections compatible with the preceding philosophy. Since fine structure is washed out by the presence of a dominant non-resonant scattering material (i.e., $\Sigma_R(u)$ becomes a smooth function of u), the case of an infinitely dilute resonance absorber or scatterer is particularly simple. Hence it is customary to define a self-shielding factor which multiplies the infinitely dilute cross section to yield the appropriate cross section for the non-dilute cases.

The preceding outline glosses over many complications. These will be addressed in more detail in the sections which follow,

Figure 2.1 Schematic Illustration of Error due to Neglecting Resonance - Induced Flux Dips

in which the following points are addressed:

- (a) accurate description of the flux dip caused by a resonance
- (b) motivation of the use of single-level Breit Wigner resonances without interference or overlap
- (c) development of prescriptions for the effective cross section and self-shielding factors.

The chapter concludes with some numerical studies related to verification of limiting case results and to examination of the functional dependence of self-shielding factors on the relative magnitude of the background scattering and on the temperature of the medium.

2.2 Intermediate Resonance Approach to Self-Shielding

Unfortunately, in the general case not all scattered neutrons are removed from under a resonance. Various approximate treatments have been devised. The narrow resonance and wide resonance approximations represent initial limiting-case attempts to deal with this difficulty.

If the average energy loss per collision is smaller than the practical width — the resonance width such that the resonance cross section is twice that of the background cross section — of the isotope in question, then one can adopt the wide resonance approximation (C1). Resonance (or background) scattered neutrons will not lose enough energy to be scattered out of the resonance and thus can interact with the resonance again. This approximation is quite good.

for low energy resonances of a heavy absorber.

On the other hand, if the practical width is much smaller than the average energy loss per collision, neutrons will be scattered out from under the resonance. This narrow resonance approximation has been useful in the presence of strongly moderating materials.

In certain cases the above-mentioned approximations fail. Some resonances behave like neither narrow nor wide resonances, rather like something in between. Goldstein accordingly proposed a new approximation, the intermediate resonance approximation (G1). In this approximation a resonance is considered to have properties of both narrow and wide resonances. To allocate the relative contributions, two new parameters are defined which characterize the slowing-down operator of the absorber and the scatterer.

These two new parameters are calculated from a pair of coupled transcendental equations by numerical iteration. The energy-dependent flux is then calculated in terms of these parameters. This calculated flux is used in computation of the resonance integral. This approach is confirmed to give very good agreement with measured resonance integral data by many investigators (G2, I1, and M1).

The intermediate resonance approximation assumes that the heavy absorber scatters as well as absorbs, and the scatterer absorption is negligible. This latter assumption is plausible for all reactor types, since the absorption in the coolant or moderator is generally kept at a minimum. Another requirement is that the

resonances are not close to sources or sinks in energy space. That is, the resonances are spaced such that the flux will recover from the effects of the resonance (i.e., Placzek oscillations). This means that the resonances are separated by $\geq 6\xi_i$, where ξ_i is the average lethargy gain per collision for isotope i . For U-238, $D \approx 20$ eV, while at 100 eV, $6\xi_i \leq 5$ eV.

In calculating the group average cross section one makes another assumption, that the resonances do not interfere with the potential scattering cross section. The potential scattering cross section is the constant scattering cross section attributable to the physical size of the nucleus. Interference between the potential scattering cross section and a scattering resonance increases the overall cross section at the high energy side of the resonance tail and decreases the overall cross section at the low energy side of the resonance tail. The effects of interference between resonance and potential scattering become appreciable at higher energies (above 10 keV), which is above the resolved resonance region of U-238.

Another assumption is to neglect the overlap of resonances. Resonances of different isotopes can overlap; the resonances of the same isotope can also overlap, known as self-overlap. Two resonances overlap when they are close enough in energy space that the cross section midway between these two resonances is influenced by both resonances. This may occur at very high temperatures due to doppler

broadening, but is not significant at reactor operating temperatures for the fertile isotopes. The overlap of two resonances of different isotopes is also not important for our purposes (G3). Therefore, in calculations of present interest, one can assume that resonances do not overlap, calculate the cross section contribution of each resonance separately, and then sum all the contributions.

Based on the above assumptions the group-averaged cross section for a nuclear interaction of type x is:

$$\bar{\Sigma}_{xg} = \frac{\int_{\Delta E} \Sigma_x(E) \phi(E) dE}{\int_{\Delta E} \phi(E) dE} \quad (2-2)$$

where $\Sigma_x(E)$ is the macroscopic cross section of the medium for nuclear interaction type x
 $\phi(E)$ is the energy dependent neutron flux in that medium

ΔE is the width of the group g .

Neglecting overlap effects, Eq (2-2) can be written as

$$\bar{\Sigma}_{xg} = \frac{\sum_{k=1}^K \int_{\Delta E} \Sigma_{x_k}(E) \phi_k(E) dE}{\int_{\Delta E} \phi(E) dE} \quad (2-3)$$

where k is the resonance number index in group g .

The sum is taken over all the resonances in the group, each weighted by the proper flux. This flux, according to the intermediate resonance approximation (G4), is:

$$\phi_k(E) = \frac{\sum_m + \lambda_k \sum_p}{\sum_m + \sum_a(E) + \lambda_k \sum_s(E)} \quad (2-4)$$

where λ_k is the intermediate resonance approximation parameter ($\lambda = 1.0$ for the narrow resonance approximation, which we will employ throughout)

$\sum_m$ is the constant moderator cross section

$\left. \begin{array}{l} \sum_a(E) \\ \sum_s(E) \\ \sum_p \end{array} \right\}$ are the resonance absorption, scattering, and potential scattering cross sections of the resonance absorber.

The appropriate formula for the cross section will be the single level Breit-Wigner formula. Multi-level formulas can also be used, but it has been shown that the use of such formulas is more applicable to the unresolved energy range and to resonance cross sections of fissile isotopes (S1). In our calculations, which deal primarily with U-238 in the resolved resonance range, the single level

formalism is adequate (B1).

Substituting the doppler-broadened single level Breit-Wigner formula without interference into Eq (2-3) along with the flux in Eq (2-4) and after some re-arrangement of the terms for the capture cross section, one obtains for the narrow resonance case:

$$\sigma_c = \sigma_p \frac{\Gamma_Y}{E_r} \frac{1}{2\Delta E} \int_{-\infty}^{\infty} \frac{\psi(t, x)}{\psi(t, x) + (\beta i)^{1/2} \chi(t, x) + \beta} dx \quad (2-5)$$

$$\text{where } \sigma_p = \sigma_{p_a} + \sigma_m \frac{N_m}{N_a} \quad (2-6)$$

$$\beta = \frac{\sigma_p}{\sigma_r} \quad (2-7)$$

$$i = \frac{\Gamma_n}{\Gamma} \frac{\sigma_{p_a}}{\sigma_r} g_J \quad (2-8)$$

$$\sigma_{s_r} = (\beta i)^{1/2} \quad (2-9)$$

$$x = \frac{2(E - E_r)}{\Gamma} \quad (2-10)$$

$$t = \frac{4E_r kT}{A\Gamma^2} \quad (2-11)$$

and σ_{p_a} is the potential scattering cross section of

the absorber

σ_m is the constant scattering cross section

$\left. \begin{array}{l} \Gamma_Y \\ \Gamma_n \\ \Gamma \end{array} \right\}$ are the capture, scattering, and total width of the resonance

$\left. \begin{array}{l} N_m \\ N_a \end{array} \right\}$ are the number densities of the coolant/clad and the absorber

E_r is the resonance energy

σ_r is the value of the cross section at the resonance peak

ΔE is the group width

t is the temperature of the medium

A is the mass of the absorber

$\left. \begin{array}{l} \psi(t,x) \\ \chi(t,x) \end{array} \right\}$ are symmetric and asymmetric Voigt shape functions (D1).

The limits of integration in Eq (2-5) are best extended from $-\infty$ to $+\infty$, even though this extension is somewhat inconsistent with neglect of overlap effects, which is the approximation being made here. Extending the limits of integration simplifies the integral and does not introduce a significant error due to the fact that the

cross section is small between two successive resonances and smaller still beyond the confines of the broad energy group.

The integral in Eq (2-5) is proportional to the $J(t, \beta, i)$ function, which is tabulated (D2, A1).

For large values of t , or in other words, for negligible Doppler broadening, this function reduces to

$$J(\infty, \beta, i) = \frac{\pi}{2\sqrt{\beta(1 + \beta - i)}} \quad (2-12)$$

For a medium composed mainly of scatterer, with few absorber atoms, $i \approx 0$ and β is large, hence

$$J(\infty, \beta, 0) = \frac{\pi}{2\beta} \quad (2-13)$$

The infinite dilution cross section for the specific group under consideration is then given by:

$$\sigma_{\infty} = \frac{\pi}{2} \sigma_r \frac{\Gamma}{E_r} \frac{1}{\Delta E} \quad (2-14)$$

There are computer codes available which calculate cross sections based on the approach described above. For example, MIDI (R1), an in-house version of IDIOT (P1), calculates resonance cross sections using the intermediate resonance approximation. Given the resonance parameters these codes calculate the intermediate resonance approximation (IRA) parameter λ_k and then the J function using the given resonance parameters and the IRA parameter. The IRA parameter modifies the J function in such a way that, as the resonance becomes narrower, the cross section becomes closer to the infinite dilution cross section.

When the IRA parameter is examined for various resonances of U-238, it is seen that most of the resonances interact like narrow resonances. Calculations carried out using the MIDI program showed that out of 457 resolved resonances only 16 have an IRA parameter more than 20 % different from the narrow resonance value, $\lambda = 1$. Therefore, when one considers the entire resonance region, one can adopt the narrow resonance approximation without appreciably affecting the value of the group average cross sections, since the contribution of these wider resonances is generally not important compared to the contribution of all the other resonances in the group (except for very low energy resonances, which are far less important in fast reactors than in thermal reactors). Based on this reasoning, we can focus our attention on the narrow resonance approximation. Also, considering the experimental uncertainty in cross sections in

the unresolved region (which is on the order of $\pm 10\%$) and the generally weak self-shielding in this region (self-shielding factor (f) values generally exceed 0.80 and are ≥ 0.95 above about 55 keV), we can further limit considerations to the resolved resonance region.

Figure 2.2 summarizes the various considerations involved in our decision to focus on resolved resonances above 100 eV.

2.3 Self-Shielding in Non-Dilute Homogeneous Media

In this section we will consider a specific case of the more general (heterogeneous) method which will be discussed in Chapter 3. As has been discussed in the preceding section, the IRA has both drawbacks and advantages. The IRA is definitely superior to the NRA when the coolant (i.e., moderator) cross section per absorber atom, σ_0 , is small. However in the FBR, σ_0 is typically in the 10 to 100 barn range. In this range the NRA yields results which are not appreciably different from those generated using the IRA (S2). Based on this observation we will restrict consideration to the NRA in calculating the effective group cross sections. As in the IRA we will assume that the flux recovers to its asymptotic value after a resonance. A neutron interacting with a resonance will either be absorbed by this resonance or will be scattered out of the small energy band which brackets the resonance. We will also assume that interference between the potential scattering and resonance cross sections

Figure 2.2 Schematic Representation of Applicable Domains for Various Phenomena and Models for U-238

and overlap are not important, as discussed in the preceding section. The interaction rate for nuclear process x in a homogeneous medium is the product of the energy-dependent macroscopic cross section and the neutron flux. Here we wish to define an energy-independent group cross section which, when multiplied by the unperturbed total flux for that group, yields the real interaction rate, that is,

$$\bar{\Sigma}_{xg} = \frac{\int_{\Delta E} \Sigma_x(E) \phi(E) dE}{\int_{\Delta E} \phi_0(E) dE} \quad (2-15)$$

where $\bar{\Sigma}_{xg}$ is the effective macroscopic group cross section for nuclear process x in group g

$\Sigma_x(E)$ is the energy-dependent cross section for nuclear process x

$\phi(E)$ is the perturbed flux

$\phi_0(E)$ is the unperturbed flux.

The difference between the perturbed and unperturbed fluxes is that the perturbed flux has fine structure due to the presence of the resonances. Unperturbed flux, on the other hand, has a smooth energy dependence (for example, a $1/E$ spectrum).

In order to calculate these two fluxes, let us review some assumptions.

(a) It has been assumed that the resonances do not overlap and that interference is not important. The assumption is a reasonable one for all resolved resonances of U-238. The interference cross section is small and its contribution to the group cross section can easily be neglected in the resolved resonance region (H1).. The overlap of resonances, as mentioned in the previous section, is not important. The observed resonance spacing for U-238 is 17.7 ± 0.7 eV and the average resonance width is about 0.03 eV (L1), therefore one does not expect overlap. Neglecting interference and overlap enables us to study each resonance separately and then combine their contributions to obtain the total cross section for the group. Based on this assumption, we will divide the energy group into still finer groups, each of which will contain only one resonance. These fine groups will be centered at the peak of the resonances, and their widths will then depend upon the integrand of the resonance integral for that resonance. The numerical integration will not be carried from $-\infty$ to $+\infty$, as done in the previous section, rather the limits will be the upper and lower bounds of the fine group. The width is chosen such that the integrand of the resonance integral at the boundary has less than 1% of the value at the maximum. Since the resonance integral depends on the densities in the medium as well as the resonance parameters, the width of this fine group will be

determined by all related parameters.

(b) The flux in this fine group will dip, due to the presence of the resonance. The amount of this dip is determined by the parameters that characterize the resonance. Figure 2.3 schematically illustrates the behavior of the flux in the presence of a resonance. As the temperature of the medium increases, the resonance broadens, thus the flux dips become shallower and wider. In Fig 2.3 the flux recovers to the asymptotic value of ϕ_0 , but if there is loss of neutrons in the resonance then the flux does not recover to its asymptotic value, but rather will be less than ϕ_0 , as shown in Fig 2.4.

It will be assumed that neutrons entering into a resonance are absorbed or scattered out of the group. This assumption is a plausible one, since the resonances of U-238 are mainly capture resonances. If a resonance energy neutron is scattered in the coolant region (or in moderator admixed with the fuel) then it will lose enough energy to be scattered out of the group, since the width of the fine group is always smaller than the mean energy loss of the neutron.

Under the above assumptions, the slowing down source past lethargy u will be constant. The number of neutrons that interact within this group will be the product of the macroscopic cross section of the medium and the neutron flux. These neutrons are supplied by the constant slowing down sources above the fine group. In other

Figure 2.3 Flux Dip due to a Resonance for Two Temperatures and No Absorption

Figure 2.4 Flux Dip due to a Resonance with Absorption and the Dependence of the Flux Dip on the Absorber Density

words, the flow of neutrons past lethargy u , $q(u)$, is equal to the product of flux per unit lethargy, $\bar{\phi}(u)$, and the removal cross section at that lethargy, $\sum_R(u)$:

$$q(u) = \sum_R(u) \bar{\phi}(u) \Delta u \quad (2-16)$$

The flux has an asymptotic value such that

$$q(u) = \xi \sum_0 \bar{\phi}_0(u) = \text{constant} \quad (2-17)$$

where ξ is the average lethargy gain per collision

$\sum_0$ is the background cross section of the medium

$\phi_0(u)$ is the unperturbed neutron flux in the medium.

Solving for the resonance neutron flux from these two equations,

$$\begin{aligned} \bar{\phi}(u) &= \frac{\xi \sum_0 \bar{\phi}_0(u)}{\Delta u \sum_R(u)} \\ &\equiv \frac{\sum_{R0}(u)}{\sum_R(u)} \phi_0(u) \end{aligned} \quad (2-18)$$

since the group removal cross section may be taken as $\sum_{R0}(u) \frac{\xi}{\Delta u}$

(G5).

This relation may be rewritten in terms of energy:

$$\bar{\phi}(E) = \frac{C_0 (E_0/E)^n}{\Sigma_R(E)} \quad (2-19)$$

where E_0 is the maximum energy of the coarse group

$$C_0 = \phi_0(E_0) \frac{\xi \sum_0 E_0}{\Delta E} = \text{constant for each energy group}$$

The exponent n in Eq (2-19) is often taken equal to unity, but here it is inserted as a parameter for greater generality. If there is no absorption in the group, then $n = 1$ and one has the familiar $1/E$ spectrum. For $n > 1$ the effect of absorption is taken into account, as seen in Fig 2.5.

Using Eq (2-19), one can calculate the unperturbed flux

$$\bar{\phi}_0(E) = \frac{C_0 (E_0/E)^n}{\sum_0} \quad (2-20)$$

Inserting Eqs (2-19) and (2-20) into Eq (2-15), we get

Figure 2.5 Effect of Absorption on the Group Flux

$$\bar{\Sigma}_x = \frac{\int \Sigma_x(E) \frac{dE}{E^n}}{\Delta E \int_R(E) \frac{dE}{E^n}} \quad (2-21)$$

where ΔE is the width of the fine group.

The microscopic effective group cross section is defined as $\bar{\Sigma}_x$ per absorber atom. Under the assumption that resonance interference is not important,

$$\bar{\sigma}_{x_g} = \sum_{j=1}^J \frac{1}{N_0} \bar{\Sigma}_{x_j} \quad (2-22)$$

where j is the number of the resonance in the energy group

J is the total number of resonances in the gth group

N_f , N_c , N_0 are the number densities of the fuel pin, coolant and resonance absorber.

Using this new definition one can write

$$\sigma_{x_g} = \frac{\sum_{j=1}^J \frac{\Delta E_j}{\left(\sigma_x(E) + \frac{N_f}{N_o} \sigma_x^n \right) / \left(\sigma_R(E) + \frac{N_c}{N_o} \sigma_R^n \right) \frac{dE}{E^n}}}{\frac{1}{\sigma} \int_{\Delta E_g} \frac{dE}{E^n}} \quad (2-23)$$

where σ is the nonresonant background removal cross section of the medium per resonance absorber nucleus (including the potential scattering cross section of the absorber).

Defining the reduced energy and temperature variables x and t as

$$x = 2 \left[\frac{E - E_{rj}}{\Gamma_j} \right] \quad (2-24)$$

$$t = \frac{4E_{rj} kT}{A\Gamma_j^2} \quad (2-25)$$

where $\left. \begin{array}{l} E_{rj} \\ \Gamma_{xj} \end{array} \right\}$ are the energy and the total width of the resonance

A is the mass number of the absorber nucleus

T is the temperature of the medium in degrees
Kelvin.

Using the single-level Breit-Wigner doppler-broadened formula for the resonance, one gets the following cross section expressions to be used in Eq (2-23):

for a scattering interaction,

$$\sigma_s(x,t) = \sigma_r \frac{\Gamma_n}{\Gamma} \psi(x,t) + \sigma_{s_r} \chi(x,t) + \sigma_{p_a} \quad (2-26)$$

for a capture reaction:

$$\sigma_c(x,t) = \sigma_r \frac{\Gamma_\gamma}{\Gamma} \psi(x,t) \quad (2-27)$$

and their total:

$$\sigma_R(x,t) = \sigma_r \psi(x,t) + \sigma_{s_r} \chi(x,t) + \sigma_{p_a} \quad (2-28)$$

where all the parameters are defined in the previous
section.

In order to demonstrate the equivalence of this result and the prescription quoted in the previous section, let us calculate the capture cross section. Inserting Eqs (2-27) and (2-28) into Eq (2-23), we get (again recognizing the limits are equivalent to $\pm\infty$ and taking $n = 1$):

$$\sigma_c = \sigma \frac{\Gamma_Y}{E_{r_j}} \frac{1}{2\Delta u} \int_{-\infty}^{\infty} \frac{\psi(x,t)}{\psi(x,t) + (\beta i)^{1/2} \chi(x,t) + \beta} dx \quad (2-29)$$

which is identical to Eq (2-5) in Section 2.3.

2.4 Cross Section Computation and CIDI

In this work the microscopic effective group cross sections for a given energy group structure were calculated using CIDI, a computer code which evaluates Eq (2-23). In this section a short introduction to the method used in CIDI will be presented; a more detailed explanation and a listing of the code can be found in Appendix A.

For a given energy group structure and resonance parameters, plus geometry and non-resonant cross sections for a two region unit cell, CIDI calculates the integrand and the limits of integration in Eq (2-23). It then integrates this equation using a numerical integration (Romberg quadrature) subroutine. The necessary Voigt shape

functions $\psi(x,t)$ and $\chi(x,t)$ are calculated using an approximation derived by Chiarella and Reichel (C2). A subroutine from a similar German program (H5) was used after an important correction was incorporated. The corrected approximate formula gave quite accurate values of the Voigt shape functions when compared to tabulated values (H6). Following the discussion of the previous section, CIDI then calculates the contribution of each resonance to the group effective cross section, and then sums over all resonances in the group to calculate the group effective cross section.

2.5 Bondarenko Set Self-Shielding f Factors

In this section we will calculate the f factors for the 26 group Bondarenko cross section set energy structure (also known as the ABBN or "Russian" set). In order to calculate f factors, one must have a set of infinite dilution cross sections for that particular energy group structure. The infinite dilution cross section as given by Eq (2-14) depends only on the resonance parameters and group lethargy width. Therefore our first task is to calculate the infinite dilution cross section for the energy groups used in the 26 group Bondarenko set using Eq (2-12), for the resolved resonance region, which in the ENDF/B data set, contains 457 resolved resonances of U-238.

To calculate the infinite dilution cross sections we divide each broad energy group into fine groups such that the value of the

integrand of the resonance integral at the group boundary is less than 1 % of the maximum value of this integrand. The tails of the resonances are included by analytically estimating their contribution to the group under study and to adjacent broad groups. This correction is not very important, not even a fraction of one per cent for the infinite dilution case, but will be more important as the temperature and/or absorber density increases.

The results of these calculations, along with Bondarenko's infinite dilution cross sections, are given in Table 2.1. It is seen that cross sections calculated by our numerical approach are within a fraction of a per cent of the analytical infinite dilution cross sections.

The difference between Bondarenko's results and our analytical results can be attributed to the increased number of resolved resonances in certain groups and to differences in the precision of the input data: the Russian results were published in 1964, while our results include ENDF/B data compiled through 1974.

Having calculated infinite dilution cross sections, we can now proceed to calculate the self-shielded cross sections at finite dilution. In order to calculate the cross sections all one needs to do is increase the absorber density and apply the same numerical method to this new case. The ratio of this new self-shielded cross section to the infinite dilution cross section gives the self-shielding f factor for the specific absorber density, i.e.:

Table 2.1

Comparison of Infinite Dilution Capture Cross Sections of U-238

Group	Upper Energy Bound	Analytical Value Eq (2-14) (barns)	Numerical Value Eq (2-23) CIDI Program (barns)	Bondarenko Set (barns)
14	2.15 keV	1.718	1.716	2.10
15	1 keV	3.582	3.575	3.60
16	465 eV	4.617	4.608	4.50
17	215 eV	20.583	20.463	17.0
18	100 eV	16.015	15.992	15.0
19	46.5 eV	55.673	55.532	58.0
20	21.5 eV	81.020	80.747	82.0
21	10 eV	169.880	169.06	171.0
(22	4.65 eV)			

$$f_{xg} = \frac{\sigma_{xg}}{\sigma_{xg\infty}} \quad (2-30)$$

where σ_{xg} is the self-shielded effective group cross section for process x of group g

$\sigma_{xg\infty}$ is the infinite dilution cross section for process x of group g .

The effects of absorber density and temperature on the self-shielding f factors calculated in this manner will be discussed in the following subsections.

2.5.1 Effects of σ_0 on f Factors

The f factor, in a strict sense, depends on all the parameters that define the total cross section of the mixture, including temperature, densities, and resonance parameters. However, all concentration-related effects are embodied in one parameter, the total cross section of non-resonance-absorber nuclei per absorber nucleus, σ_0 . Since σ_0 must account for a rather complex combination of effects, its use raises some ambiguity in f factor calculations (S3).

The general dependence of the f factor on σ_0 has not been formulated in closed analytical form. However, there is an approximate relation between σ_0 and the f factor, strictly applicable

only at zero temperature (S3):

$$f \approx \left[\frac{\sigma_p + \sigma_o}{\sigma_r + \sigma_p + \sigma_o} \right]^{1/2} \quad (2-31)$$

where σ_o is as previously defined

σ_p is the potential cross section of the
resonance absorber

σ_r is the cross section at the resonance peak

Other researchers have used actual self-shielding calculations and have curve-fit their results to obtain empirical relations between f and σ_o , such as (L2):

$$f = A \tanh (B (\ln \sigma_o + C)) + D \quad (2-32)$$

where A , B , C , and D are constants determined by four values of f at given σ_o values.

Using the formulation in Eq (2-31) one finds that $\frac{1}{1-f^2}$ should be a linear function of σ_o .

Tables of f factors were calculated for the same σ_0 values as in the Bondarenko set. The results of these calculations, including temperature dependence, will be given at the end of this section. At this point, note Fig 2.6, which shows how f values (in the form $\frac{1}{1-f^2}$) vary with σ_0 for two different energy groups. Based on the essentially linear dependence illustrated, the f factor for an energy group and any desired σ_0 value can be calculated given two f values for this energy group at two different σ_0 values.

It is wise, however, not to overdo reliance on this apparent near-linearity. In the worst case (lowest energy groups) errors up to 30% can result; on the other hand, given σ_0 values bracketing the desired entry, this method of interpolation can produce results accurate to within better than $\pm 3\%$ for intermediate and high energy groups.

2.5.2 Effects of Temperature on f Factors

The effects of temperature on resonances (the doppler effect) have been studied exhaustively over the past several decades. An increase in temperature broadens a resonance and thus reduces its effectiveness for self-shielding. Therefore one expects to see an increase in f factors as temperature increases. An increase in the slope of the curves given in Fig 2.6 is also expected as temperature increases.

Figure 2.6 Typical Variation of f with σ_0

Calculations have been made at three temperatures. The results, including the results of the previous sub-section, are given in Tables 2.2 and 2.3. When these results are compared with Bondarenko's results, one observes that the f factors behave in a very similar way with respect to changes in temperature or σ_0 . Part of the discrepancy between Bondarenko's results and ours may be attributed to the larger number of resolved resonances and more accurate data used in the present work.

The temperature coefficient of a resonance cross section, based on analysis of the doppler effect is (H2):

$$\frac{1}{\sigma} \frac{d\sigma}{dT} \propto T^{-n} \quad (2-33)$$

where the value of n is determined from measured (or computed) values of the temperature coefficient (N1).

For a given value of σ_0 , f should therefore be a linear function of $\ln T$. This correlation was confirmed, and accurately predicts f factors for any intermediate temperatures. In Fig 2.7 this relation is illustrated for two representative groups.

Table 2.3

f_s Factors for Bondarenko Set Group Structure
in the Resolved Resonance Region

- Elastic Scattering Cross Section Self-Shielding Factors for U-238 -

Group	Temp °K	σ_0	=	10^4	10^3	10^2	10^1	0
13	300.			0.994	0.956	0.821	0.705	0.686
	600.			0.995	0.964	0.840	0.718	0.694
	1200.			0.996	0.971	0.860	0.733	0.707
14	300.			0.989	0.921	0.740	0.627	0.598
	600.			0.991	0.935	0.762	0.638	0.605
	1200.			0.993	0.948	0.786	0.651	0.614
15	300.			0.982	0.877	0.658	0.554	0.530
	600.			0.985	0.899	0.682	0.563	0.536
	1200.			0.990	0.920	0.710	0.575	0.544
16	300.			0.979	0.874	0.714	0.652	0.639
	600.			0.984	0.894	0.729	0.657	0.642
	1200.			0.988	0.914	0.748	0.664	0.647
17	300.			0.811	0.449	0.229	0.177	0.163
	600.			0.842	0.481	0.235	0.178	0.163
	1200.			0.873	0.528	0.245	0.180	0.164
18	300.			0.877	0.604	0.459	0.424	0.416
	600.			0.902	0.634	0.465	0.425	0.417
	1200.			0.923	0.669	0.475	0.427	0.418
19	300.			0.947	0.294	0.176	0.146	0.138
	600.			0.692	0.312	0.177	0.146	0.139
	1200.			0.740	0.339	0.180	0.146	0.139
20	300.			0.783	0.432	0.316	0.288	0.281
	600.			0.840	0.455	0.319	0.288	0.281
	1200.			0.823	0.485	0.324	0.289	0.282
21	300.			0.850	0.627	0.547	0.514	0.508
	600.			0.872	0.642	0.550	0.514	0.508
	1200.			0.895	0.661	0.553	0.514	0.508

Figure 2.7 Representative Dependence of f_c on $\ln T$ for U-238 Capture

2.6 f Factors for the FTR-300 Set

Similar calculations were carried out using the group structure of the FTR-300 30 group set. Instead of reproducing the entire f factor table for this case, we concentrated our efforts on only two σ_0 values, 20 and 100, since most LMFBR blankets can be simulated by media with σ_0 between these two values. We also did calculations for various temperatures. The results of these calculations were all qualitatively similar to those discussed in the previous section. Therefore, without going into any detail, we will just present the results, in Tables 2.4 and 2.5. Figures 2.6 and 2.7 compare selected results from the present work, from Bondarenko, and from FTR-300.

2.7 Conclusion

In this chapter the concept of energy self-shielding in a homogeneous medium has been reviewed. Prescriptions developed in the past by other investigators were re-examined. Justification was presented for limiting consideration to narrow, isolated Breit Wigner resonances. Calculated self-shielding factors were then shown to be in good agreement with those of other authors. The next step involves introduction of the effects of heterogeneity. Here we will depart from past practice.

Table 2.4

f_c Self-Shielding Factors for FTR-300 Group Structure
 - Capture Cross Section Self-Shielding Factors for U-238 -

Group	Temp °K	σ_0	=	100.0	20.0
<hr/>					
18	300.			0.741	0.530
	600.			0.785	0.581
	1200.			0.826	0.636
19	300.			0.798	0.608
	600.			0.835	0.663
	1200.			0.869	0.717
20	300.			0.673	0.476
	600.			0.722	0.521
	1200.			0.765	0.570
21	300.			0.706	0.502
	600.			0.749	0.552
	1200.			0.791	0.604
22	300.			0.629	0.420
	600.			0.676	0.467
	1200.			0.724	0.519
23	300.			0.511	0.314
	600.			0.562	0.353
	1200.			0.616	0.398
24	300.			0.456	0.259
	600.			0.511	0.297
	1200.			0.571	0.342
25	300.			0.398	0.221
	600.			0.448	0.254
	1200.			0.503	0.294
26	300.			0.209	0.110
	600.			0.235	0.123
	1200.			0.267	0.139
27	300.			0.111	0.054
	600.			0.124	0.058
	1200.			0.142	0.064
28	300.			0.059	0.032
	600.			0.062	0.032
	1200.			0.067	0.033
29	300.			0.074	0.037
	600.			0.077	0.038
	1200.			0.083	0.039
<hr/>					

Table 2.5

f_s Self-Shielding Factors for FTR-300 Group Structure
 - Elastic Scattering Cross Section Self-Shielding Factors for U-238 -

Group	Temp °K	σ_0	=	100.0	20.0
18	300.			0.888	0.728
	600.			0.860	0.748
	1200.			0.882	0.771
19	300.			0.874	0.794
	600.			0.889	0.808
	1200.			0.904	0.824
20	300.			0.749	0.637
	600.			0.772	0.653
	1200.			0.798	0.673
21	300.			0.778	0.681
	600.			0.798	0.695
	1200.			0.820	0.713
22	300.			0.717	0.619
	600.			0.739	0.632
	1200.			0.764	0.649
23	300.			0.658	0.564
	600.			0.682	0.577
	1200.			0.709	0.595
24	300.			0.711	0.634
	600.			0.734	0.646
	1200.			0.760	0.661
25	300.			0.727	0.680
	600.			0.740	0.686
	1200.			0.756	0.694
26	300.			0.341	0.292
	600.			0.349	0.295
	1200.			0.360	0.299
27	300.			0.249	0.207
	600.			0.256	0.209
	1200.			0.266	0.212
28	300.			0.219	0.194
	600.			0.221	0.194
	1200.			0.224	0.195
29	300.			0.812	0.804
	600.			0.813	0.804
	1200.			0.814	0.804

CHAPTER 3

UNIT CELL FLUXES

In the previous chapter the energy self-shielding in a homogeneous medium was examined. In this chapter, groundwork will be prepared to study self-shielding in a heterogeneous medium. The heterogeneous effective group cross section will be derived and from this derivation the need for region-wise unit cell fluxes will become self-evident. The dependence of these fluxes on various cell parameters will also be investigated for some limiting cases amenable to simple analytic formulations. Finally, these analytic formulations will be checked using numerical methods.

3.1 Calculation of Heterogeneous Group Cross Sections

The heterogeneous macroscopic group cross section is obtained by rewriting Eq (2-2), of the previous chapter, for a heterogeneous medium:

$$\bar{\Sigma}_{x_k} = \frac{\int_{V_{\text{cell}}} d\underline{r} \int_{\Delta E} \Sigma_x(\underline{r}, E) \phi(\underline{r}, E) dE}{\int_{V_{\text{cell}}} d\underline{r} \int_{\Delta E} \phi_{\text{cell}}(\underline{r}, E) dE} \quad (3-1)$$

where $\left. \begin{array}{l} \Sigma_x(\underline{r}, E) \\ \phi(\underline{r}, E) \end{array} \right\}$ are the position and energy dependent macroscopic cross section and the flux

$\phi_{\text{cell}}(\underline{r}, E)$ is the unperturbed cell flux

V_{cell} is the volume of the heterogeneous unit cell, composed of fuel and coolant regions.

The position-dependent flux and the cross section will be identified as belonging to the fuel or coolant region by a subscript f or c, respectively. Using this identification, and assuming that the cross sections are position-independent in each region, Eq (3-1) can be written as:

$$\bar{\Sigma}_{x_k} = \frac{\int_{\Delta E} dE \Sigma_{x_f}(E) \int_{V_f} d\underline{r} \phi_f(\underline{r}, E) + \int_{\Delta E} dE \Sigma_{x_c}(E) \int_{V_c} d\underline{r} \phi_c(\underline{r}, E)}{\int_{V_{\text{cell}}} d\underline{r} \int_{\Delta E} \phi_{\text{cell}}(\underline{r}, E) dE} \quad (3-2)$$

The explicit position dependence of the flux in the coolant and fuel regions is not really necessary for these calculations. A simpler prescription can be obtained by defining a volume-average flux:

$$\bar{\phi}_{\alpha}(E) = \frac{1}{V_{\alpha}} \int_{V_{\alpha}} d\underline{r} \phi_{\alpha}(\underline{r}, E) \quad (3-3)$$

where the α subscript stands for either fuel or coolant, as appropriate.

With the use of Eq (3-3), Eq (3-2) reduces to

$$\sum_{x_k} = \frac{\int_{\Delta E} \left\{ V_f \Sigma_{x_f}(E) \bar{\phi}_f(E) + V_c \Sigma_{x_c}(E) \bar{\phi}_c(E) \right\} dE}{\int_{\Delta E} V_{\text{cell}} \bar{\phi}_{\text{cell}}(E) dE}$$

Here $\bar{\phi}_{\text{cell}}(E)$ is the unperturbed cell flux, which is the same as the unperturbed homogeneous flux.

In order to calculate $\bar{\Sigma}_{x_u}$ using Eq (3-4), two quantities

are necessary: $\bar{\phi}_f(E)$ and $\bar{\phi}_c(E)$. Each of these fluxes must be known: either separately, or in the form of one flux and a ratio of the two fluxes. We will adopt the latter approach and consider the fuel flux and the ratio of the coolant flux to the fuel flux. As will be shown, the ratio of the volume-averaged fluxes depends on the optical thickness of the media and the partitioning of the total neutron source between fuel and coolant. The flux ratio is then defined by

$$R \equiv R(Q, \tau_f(E), \tau_c(E)) = \frac{\bar{\phi}_c(E)}{\bar{\phi}_f(E)} \quad (3-5)$$

where Q is the fraction of the total neutron source introduced in one of the two media
 $\tau(E)$ is the optical thickness of the coolant (c)
 or fuel (f).

With Eq (3-5), Eq (3-4) can be written as

$$\bar{\Sigma}_{x_u} = \frac{\int_{\Delta E} \left\{ V_f \Sigma_{x_f}(E) + V_c \Sigma_{x_c}(E) R \right\} \bar{\phi}_f(E) dE}{V_{\text{cell}} \int_{\Delta E} \bar{\phi}_{\text{cell}}(E) dE} \quad (3-6)$$

The volume-averaged fuel flux can be calculated from a neutron balance between source and removed neutrons. Consider a fine group narrow enough such that all interactions (scattering or absorption) remove a neutron from the group (i.e., narrow resonance approximation):

$$q(u) = \sum_{R_f} V_f \bar{\phi}_f \Delta u + \sum_{R_c} V_c \bar{\phi}_c \Delta u \quad (3-7)$$

where Σ_R is the removal cross section of the particular region in the cell.

The slowing down density and the unperturbed or asymptotic flux (flux just above the resonance or at the resonance in the absence of resonance interactions) is given by

$$q(u) = \xi \Sigma_0 \bar{\phi}_0(u) \quad (3-8)$$

where ξ is the average lethargy gain per collision

Σ_0 is the background cross section of the cell
(volume-weighted homogenized cross
section just above the resonance)

$\phi_0(u)$ is the unperturbed flux at a reference lethargy.

From Eqs (3-7) and (3-8), with the use of Eq (3-5), the fuel flux is calculated

$$\bar{\phi}_f(u) = \frac{\frac{\xi}{\Delta u} \sum_0 \bar{\phi}_0(u)}{\sum_{R_f} (u) v_f + \sum_{R_c} (u) v_c R} \quad (3-9)$$

This relation may also be written in terms of the energy variable:

$$\bar{\phi}_f(E) = \frac{C_0 (E_{\max}/E)^n}{\sum_{R_f} (E) v_f + \sum_{R_c} (E) v_c R} \quad (3-10)$$

Where we allow for an E^{-n} variation in the asymptotic flux within a broad group whose upper energy is $E_{\max}$, as is customary. As will be seen, the normalization, here expressed in the role of C_0 , is arbitrary.

Inserting Eqs (3-10) and (2-20) into Eq (3-6), the group cross section is calculated:

$$\bar{\Sigma}_{x_k} = \frac{\int_{\Delta E} \frac{V_f \int x_f (E) + V_c \int x_c (E) R}{\int_{R_f} (E) V_f + \int_{R_c} (E) V_c R} \frac{dE}{E^n}}{V_{cell} \int_{\Delta E} \frac{1}{\Sigma_{R_{cell}}} \frac{dE}{E^n}} \quad (3-11)$$

where $\Sigma_{R_{cell}}$ is the non-resonance removal cross section of the homogenized cell.

If the resonance absorber is only in the fuel region and the coolant cross section is energy independent, Eq (3-11) reduces to

$$\bar{\Sigma}_{x_k} = \frac{\int_{\Delta E} \frac{\int x_f (E)}{\int_{R_f} (E) + \frac{V_c}{V_f} \int_{R_c} R} \frac{dE}{E^n}}{\int_0^1 \int_{\Delta E} \frac{dE}{E^n}} \quad (3-12)$$

which reduces to Eq (2-15), the homogeneous version, if $R = 1$.

Therefore the effect of heterogeneity is introduced into the cross section expression via the flux ratio R . Indeed, we could have developed Eq (3-12) from Eq (2-21) directly by the physical

observation that heterogeneity merely creates an imbalance in the relative removal rates by fuel and coolant, favoring the latter by the ratio of coolant to fuel fluxes, R . The rest of this chapter will deal with the method of calculating the flux ratio, R , in a unit cell.

3.2 Unit Cell Description

Unit cells of interest in reactor physics are either square or hexagonal, as shown in Fig 3.1. While a unit cell normally contains three physically distinct regions: fuel, clad, and coolant, in these calculations a two-region cell will be considered: The clad region will be homogenized with the coolant region. Combining two regions into one will not influence the final results appreciably in a FBR unit cell (G6).

To solve for the fluxes in the unit cell, the Wigner-Seitz cylindricalization method may be used, in which the square or hexagonal cell is replaced by a cylindrical cell having the same cross section area (W1).

Mirror (specular reflection) or white (diffuse reflection) boundary conditions may be used at the outer periphery of the cell. Mirror boundary conditions, when used with diffusion theory, result in little error, but the error can become appreciable when transport theory is employed, as discussed below (N2).

Square Lattice

Hexagonal
Lattice

Cylindricized Cell

Area equal to square cell shown above

Orbit of Trapped Neutron

Figure 3.1 Unit Cell of Square and Hexagonal Lattices
and their Cylindricized Representation

Calculations of tight lattices in thermal reactors first brought to attention problems with mirror boundary conditions in cylindrical geometry (H3). Since all fast reactor lattices are also tight, that is, the lattice spacing is much smaller than the neutron mean free path, similar problems would also be expected to occur in fast reactor core or blanket unit cell calculations. This boundary condition was shown to lead to over-estimation of the coolant flux because neutrons emitted at certain angles in the coolant region can never enter the fuel region (see Fig 3.1); they are trapped in orbits which remain forever in the coolant. In the true physical lattices, however, neutrons need only traverse several rows of fuel rods before entering a fueled region. Furthermore, this class of events is relatively unimportant in cells made of good diffusive media where the mean free path of the neutrons is much smaller than the cell dimensions, since the medium itself redistributes neutrons (almost isotropically) through successive collisions. For this reason, the mirror boundary condition often works well when diffusion theory is applicable. As we have noted, diffusion theory is not applicable to unit cells of fast systems, and hence the mirror boundary condition can lead to significant errors (F1).

The other common choice for a boundary condition is the white boundary condition, which returns all neutrons from the boundary with an isotropic distribution. It has been shown that the white boundary condition underestimates the flux variation in the

cell by forcing the angular flux in the cell to be almost isotropic anywhere (P2). When the results of mirror and white boundary conditions are compared, it has been found that the white boundary condition results in less error than the mirror boundary condition (G6). Based on this finding, white boundary conditions will be used in our numerical calculations wherever the necessity of using a cylindrical cell arises. This difficulty also motivates reliance on methods which treat exact geometries without the need for cylindricalization.

3.3 Calculation of Flux Ratio

Although we will employ more sophisticated methods in a subsequent section of this chapter, it is highly useful to attack the problem of determining the unit cell flux ratio using some simple analytical methods. In this section we will employ an integral equation/kernel method approach, and in Section 3.4 an escape probability method will be employed. These approaches will provide two very useful results: a clue as to appropriate functional relations for correlating results obtained using the more complicated numerical methods and exact results for some limiting cases.

The transport equation for the neutron flux in a medium with isotropic neutron birth and scattering sources is the Peierls' Equation (C3, G7):

$$\phi(\underline{r}) = \int_V G(\underline{r}/\underline{r}') [q(\underline{r}') + \Sigma_s \phi(\underline{r}')] d\underline{r}' \quad (3-13)$$

where $\left. \begin{array}{l} \phi(\underline{r}) \\ \phi(\underline{r}') \end{array} \right\}$ are the fluxes at vector points $\underline{r}$ and $\underline{r}'$

$q(\underline{r}')$ is the source at $\underline{r}'$

V is the volume of the cell

$G(\underline{r}/\underline{r}')$ is the first flight kernel giving the
uncollided flux at $\underline{r}$ due to a unit
isotropic source at $\underline{r}'$.

Under the flat flux approximation, Eq (3-13) can be expressed in terms of volume averaged fluxes and kernels. One obtains a coupled set of equations for the coolant and fuel average fluxes:

$$\bar{\phi}_c = K_{cc}[Q_c + \Sigma_{sc} V_c \bar{\phi}_c] + K_{cf}[Q_f + \Sigma_{sf} V_f \bar{\phi}_f] \quad (3-14)$$

$$\bar{\phi}_f = K_{fc}[Q_c + \Sigma_{sc} V_c \bar{\phi}_c] + K_{ff}[Q_f + \Sigma_{sf} V_f \bar{\phi}_f] \quad (3-15)$$

where

$$Q_{\alpha} = \frac{1}{V_{\alpha}} \int q_{\alpha}(\underline{r}) d\underline{r} / Q_T \quad (3-16)$$

fraction of initial neutron source in region Q

$$Q_T = Q_c + Q_f \quad (3-17)$$

total neutron source

$$K_{\alpha\beta} = \int_{V_{\alpha}} d\underline{r} \int_{V_{\beta}} G(\underline{r}/\underline{r}') d\underline{r}' \quad (3-18)$$

and from the reciprocity theorem,

$$K_{cf} = K_{fc} \quad (3-19)$$

This approach was first studied by Corngold (C4) for planar geometry; an infinite set of coupled integral equations was obtained by expanding the fluxes into orthogonal polynomials in space and angular coordinates. The kernels given by Eq (3-18) were also calculated analytically for small values of the optical thickness of the fuel lump. The same approach has been used in cylindrical geometry to calculate the resonance integral (T1) and the ratio of the moderator to fuel fluxes (F2). For the source-in-coolant case the kernels were also evaluated for small optical

thicknesses by these authors.

Here we generalize the above-mentioned methods by introducing sources in both regions and considering any values of the optical thicknesses of the lump. Solving for the ratio of $\bar{\phi}_c/\bar{\phi}_f$ from Eqs (3-14) and (3-15) and rearranging the coefficients, one obtains:

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 + \left[\frac{K_{cc}}{K_{cf}} - 1 \right] + \left[K_{cf} - \frac{K_{cc}K_{ff}}{K_{cf}} \right] \left[\sum_s v_f \right] Q_c}{1 + \left[\frac{K_{ff}}{K_{cf}} - 1 \right] + \left[K_{cf} - \frac{K_{cc}K_{ff}}{K_{cf}} \right] \left[\sum_s v_c \right] Q_f} \quad (3-20)$$

In the present work we can further simplify Eq (3-20), since all interactions are assumed to remove neutrons from the group. Thus, all interactions are effectively "absorption" and there is no scattering, or $\Sigma_s = 0$. Hence

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 + \left[\frac{K_{cc}}{K_{cf}} - 1 \right] Q_c}{1 + \left[\frac{K_{ff}}{K_{cf}} - 1 \right] Q_f} \quad (3-21)$$

Actually, as we will show later, for scattering optical thickness in the region of interest, scattering has practically no effect on the flux ratio, and Eq (3-21) is more generally applicable.

For any value of the optical thickness, the kernels in Eq (3-20) are complicated functions of the fuel and coolant cross sections. However, simple analytical expressions for these kernels can be derived for some limiting values of the fuel and coolant optical thicknesses. These special limiting cases will be studied in the following sections.

3.4 Calculation of Flux Ratio via Escape Probabilities and Partial Currents

An alternative formulation of the problem addressed in the preceding section can be developed in terms of escape probabilities. This approach was taken by Gregory (G6) and here only results will be given. In order to calculate the flux ratio of the unit cell the following probabilities are defined:

- p_1 = escape probability of a neutron born in fuel
- p_2 = escape probability of a neutron born in coolant
- P_1 = escape (penetration) probability of a neutron entering
the fuel
- P_2 = escape (penetration) probability of a neutron entering
the coolant

j^+ = current entering fuel region

j^- = current entering coolant region

One calculates the current entering the fuel region due to a uniform source per unit volume, S_1 , in the fuel region. The first generation neutrons, those which cross the fuel-coolant boundary, give rise to first generation current. Similar calculations are done for second, third, etc., generation neutrons, giving rise to higher generation currents. Then similar calculations are applied to generate the partial currents due to a uniform source per unit volume, S_2 , in the coolant region. The final partial currents due to neutrons of all generations are

$$j^+ = S_1 P_1 \frac{r_1}{2} \left[\frac{P_2}{1 - P_2 - P_1 P_2} \right] + S_2 P_1 \frac{1}{2} \left[\frac{r_2^2 - r_1^2}{r_1} \right] \left[\frac{1}{1 - P_2 - P_1 P_2} \right] \quad (3-22)$$

$$j^- = S_1 P_1 \frac{r_1}{2} \left[\frac{1 - P_2}{1 - P_2 - P_1 P_2} \right] + S_2 P_2 \frac{1}{2} \left[\frac{r_2^2 - r_1^2}{r_1} \right] \left[\frac{1}{1 - P_2 - P_1 P_2} \right] \quad (3-23)$$

where r_1 is the radius of the fuel rod

r_2 is the radius of the cylindricized cell boundary.

The statement of neutron balance in the two regions of the cell enables one to calculate the region-wise average fluxes:

$$\sum_{af} \bar{\phi}_f \pi r_1^2 = 2\pi r_1 (j^+ - j^-) + \pi r_1^2 S_1 \quad (3-24)$$

and

$$\sum_{ac} \bar{\phi}_c \pi (r_2^2 - r_1^2) = 2\pi r_1 (j^- - j^+) + \pi (r_2^2 - r_1^2) S_2 \quad (3-25)$$

or

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{r_2^2 - r_1^2}{r_1^2} \frac{\sum_{ac} 2r_1 (j^- - j^+) + (r_2^2 - r_1^2) S_2}{\sum_{af} 2r_1 (j^+ - j^-) + r_1^2 S_1} \quad (3-26)$$

where $\bar{\phi}_\alpha$ is the regionwise volume averaged flux of
region α

$\sum_{a\alpha}$ is the macroscopic absorption (removal) cross
section of region α

Inserting Eqs (3-22) and (3-23) into Eq (3-26) with

$$Q_f = \frac{S_1 r_1}{S_1 r_1 + S_1 z_2} = \frac{S_1 V_1}{S_1 V_1 + S_2 V_2} \quad (3-27)$$

$$\text{where } z_2 = (r_2^2 - r_1^2)/r_1$$

one gets,

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{\tau_2 p_1 (1 - P_2)}{\tau_1 p_2 (1 - P_1)} \left[\frac{1 + \frac{[1 - P_1 P_2 - p_2 (1 - P_1) - p_1 (1 - P_2)] Q_c}{p_1 (1 - P_2)}}{1 + \frac{[1 - P_1 P_2 - p_1 (1 - P_2) - p_2 (1 - P_1)] Q_f}{p_2 (1 - P_1)}} \right] \quad (3-28)$$

After some algebraic manipulations the relations between escape probabilities and the kernels used in Eq (3-21), for $\Sigma_{sf} \approx 0$, can be seen to be:

$$K_{cf} = \tau_1 p_2 (1 - P_1) = \tau_2 p_1 (1 - P_2) = K_{fc} \quad (3-29a)$$

$$K_{cc} = [1 - P_2 - P_1 P_2 - p_2 (1 - P_2) + p_1 (1 - P_2) (\tau_2 - 1)] \tau_2 \quad (3-29b)$$

$$K_{ff} = [1 - P_2 - P_1 P_2 - p_1 (1 - P_2) + p_2 (1 - P_2) (\tau_1 - 1)] \tau_1 \quad (3-29c)$$

where τ_1 and τ_2 are the optical thicknesses of the
 fuel and coolant region,
 respectively.

The preceding development will be used to determine the
 flux ratios for some limiting cases in the following section.

3.5 Limiting Cases

3.5.1 Dependence on Source Ratio

For the case of optically thin coolant (which approaches
 the case of present interest — the FBR unit cell), Eq (3-21)
 reduces to

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = 1 + A Q_c = 1 + A(1 - Q_f) \quad (3-30)$$

As can be seen from Eq (3-30), the flux ratio is a linear
 function of the fraction of the total source born in the fuel (or
 coolant); when all neutrons are born in the fuel, the flux ratio is
 unity and when all neutrons are born in the coolant, the flux ratio
 is a maximum.

This linear functional dependence is an important attribute
 of any model to be used for FBR unit cells. In LWR's the slowing

down source is almost entirely in the coolant, $Q_c \approx 1.0$, and the limiting case of the maximum flux ratio applies. If this were to be carried over to the FBR case a serious error would result, since the oxygen in UO_2 contributes a significant elastic slowing down source, and Q_f is therefore appreciable - on the order of 0.4 - and hence this factor must be taken into account. This also illustrates the danger of adopting thermal reactor prescriptions for FBR's without careful examination of the underlying assumptions.

3.5.2 Dependence of Flux Ratio on Optical Thickness:

The next specific case to be considered involves weakly absorbing fuel and coolant. In this case we can use the escape probability method (Eq. (3-28)) to derive an appropriate limiting expression.

To evaluate escape probabilities we need the escape and penetration chords. Gregory (G6) has derived an expression for the latter in the case of a cylinder, $\bar{L} = 8V/3S$; while the Dirac penetration chord is shown to be $\bar{L} = 4V/S$ in many texts (C5, M2).

First order approximations for the escape probabilities p_1 and P_1 , defined in Section 3.4, for the fuel rod characterized by $\tau_{af} = \int_{af} \bar{L}_f$ are given by:

$$p_1 = 1 - \frac{2}{3}\tau_{af} + \dots \quad (3-31)$$

$$P_1 = 1 - \tau_{af} + \frac{2}{3}\tau_{af}^2 + \dots \quad (3-32)$$

For the annular coolant region the average chord lengths are

$\bar{L}_c = 4/3z_2$ and $L_c = 2z_2$, where $z = (r_2^2 - r_1^2)/r_1$. Hence p_2

and P_2 are obtained by replacing τ_{af} by τ_{ac} in Eqs (3-31)

and (3-32). Inserting escape probabilities into Eq (3-28) and

after considerable algebraic manipulation, one finds, to first order,

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 + \frac{1}{3}\tau_{af}Q_c}{1 + \frac{1}{3}\tau_{ac}Q_f} \quad (3-33)$$

Hence when all sources are in the coolant, the flux ratio is a linear function of the optical thickness of the fuel rod, with a slope of 1/3:

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = 1 + \frac{1}{3}\tau_{af} \quad (3-34)$$

This approximate flux ratio relationship was checked for various unit cells and for fuel optical thicknesses up to ~ 0.05 and found to be in good agreement with S_8 ANISN results (G6).

As the optical thickness of the fuel increases, higher order terms in the escape probabilities would have to be taken into account.

We can instead treat the case of a completely transparent coolant and an optically black rod in a simple direct derivation as follows.

Flux is defined as track lengths per unit volume (per unit time). The flux in the coolant is then the coolant escape chord length, $\bar{\ell}_f$, per unit volume, and flux in the fuel is the absorption mean free path, λ_{af} , per unit volume:

$$\bar{\phi}_f = \frac{\lambda_{af}}{V_f} = \frac{1}{\Sigma_{af} V_f} \quad (3-35)$$

$$\bar{\phi}_c = \frac{\bar{\ell}_{ec}}{V_c} = \frac{\frac{2}{3} \bar{\ell}_{pc}}{V_c} = \frac{\frac{2}{3} \bar{\ell}_{pf}}{V_f} \quad (3-36)$$

where $\bar{\ell}_e$ is the average escape chord length from the coolant*

$\bar{\ell}_p$ is the average penetration chord length for the fuel.

*For the reader who is uncomfortable with the assumption that $\bar{\ell}_{ec} = \frac{2}{3} \bar{\ell}_{pc}$ for the irregular coolant region geometry, it is suggested that the derivation of the reciprocal case be considered (reverse the roles of fuel and coolant), in which case the coolant region is now a cylinder, for which this relationship is easily proven.

Recalling $\ell_p = 4V/S$, the flux ratio is then

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{2}{3} \tau_{af} \quad (3-37)$$

(for large τ_{af} ; i.e., $\tau_{af} \gg 1$).

From these two limits one can visualize the flux ratio as a function of the fuel optical thickness; when all the sources are in the coolant, the slope of $\bar{\phi}_c/\bar{\phi}_f$ versus fuel optical thickness varies from 1/3 to 2/3 as τ_{af} increases.

3.5.3 A Simple Flux Ratio Relation

In order to show how the flux ratio varies with the optical thickness of the fuel, all sources in the unit cell were taken in the coolant region in the preceding subsection. This reduces Eq (3-21) to a simple form where the effects of coolant optical thickness disappear. In actual cases the more general result, Eq (3-21), will apply. Generally, in fast reactor unit cells the coolant+clad optical thickness does not exceed 0.4, which enables one to use the small optical thickness limit for the coolant; i.e., the slope of 1/3 applies instead of the optically thick slope of 2/3.

Since we are interested in fuel resonance absorption, where τ_{af} can be quite large (on the order of 10^2), this leads us to propose a simple semi-empirical form of the flux ratio to be used in FBR unit cell calculations:

$$R = \frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 + \omega \tau_{af} Q_c}{1 + \frac{1}{3} \tau_c Q_f} \quad (3-38)$$

$$\text{where } \frac{1}{3} \leq \omega \leq \frac{2}{3} .$$

Equation (3-38) will be used later to develop a simple prescription for heterogeneous self-shielding factors. However, we will first carry out some extensive numerical tests of this relationship in Section 3.7. Note that the best value of ω to be used in Eq (3-38) is at present ill-defined; in the wings of a resonance a slope of $1/3$ would be more appropriate, while near the peak, a slope of $2/3$ would be more appropriate. If both regimes are important then a variable $f(\tau_{af})$ must be employed. Numerical tests will be required to select the most appropriate case.

3.6 Calculation of the Flux Ratio Using the Conventional IRA-NRA Method

One of the conventional approaches (IRA) to energy self-shielding was mentioned in Section 2.2. In this section we will examine this theory in the light of our prior discussion of flux ratios.

The formulation presented by Henry or by Goldstein (in H4 and G4) will be heavily relied upon and it is recommended that the reader consult the references for appropriate details.

The fuel and coolant fluxes in a unit cell can be calculated from the integral form of the transport equation, under the assumption of isotropic scattering. Furthermore, these fluxes can be calculated in terms of fuel and coolant escape probabilities and cross sections (H4).

We will consider a fast reactor unit cell where the fuel is very nearly black and the coolant is very nearly transparent. Further, we assume that all neutron interactions remove neutrons from the differential energy band in which that interaction took place. Under these assumptions, using the notation given in (H4), all fuel interactions may be treated as absorption (removal), i.e.,

$$\sum_{sf}^p, \sum_{sf} (E) \ll \sum_{af} (E)$$

or

$$\sum_{sf}^p \approx 0, \quad \sum_{sf} (E) \approx 0$$

With these special values for the region cross sections, and recognizing that this case is the narrow resonance approximation in Goldstein's method, we obtain for the flux ratio, by a straightforward manipulation of either author's presentation (for example, starting with Henry's Eqs (5.5.24) and (5.5.25)):

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 - P_c \tau_{af}}{P_c \tau_{ac}} \quad (3-39)$$

Using the equivalence relation relating region escape probabilities:

$$\sum_c V_c P_c = \sum_f V_f P_f \quad (3-40)$$

or in terms of optical thickness,

$$\tau_c P_c = \tau_f P_f \quad (3-41)$$

an alternative version can be obtained:

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1}{P_f} - \frac{\tau_{af}}{\tau_{ac}} \quad (3-42)$$

Using the approximate relation $P_m \approx 1 - \frac{2}{3} \tau_{am}$, applicable for small values of τ_{am} , the flux ratio of Eq (3-39) reduces to

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} \approx \frac{2}{3} \tau_{af} \quad (3-43)$$

This final result is in agreement with both the theoretical (Eq (3-37)) and with the semi-empirical (Eq (3-38)) flux ratios developed previously for the $\tau_{ac} \ll 1$, $\tau_{af} \gg 1$ limit. It should be noted, however, that conventional methods are based on use of Eq (3-42) instead of the equivalent form, Eq (3-39). The Wigner rational approximation is typically introduced for the fuel escape probability:

$$P_f = \frac{S}{S + \sigma} \quad (3-44)$$

where

$$S = \frac{a(1 - C)}{N_0 \bar{\ell}_0}$$

and where, following Goldstein's notation,

a is the Levine factor (L3)

C is the Dancoff factor (R2)

N_0 } are the number density and the mean chord length
 $\bar{\ell}_0$ } of the fuel resonance absorber.

The Dancoff factor is a function of the optical thickness of the coolant and is

$$C \approx 1 - \tau_{am} \quad (3-46)$$

for small τ_{am} (L4).

The Levine factor, a , becomes 1.0 at higher optical thicknesses (01), which applies to the fuel in the present instance.

With Eqs (3-46), (3-45), (3-44), (3-42), and $a = 1$,

one obtains:

$$\frac{\bar{\phi}_c}{\bar{\phi}_f} = 1 + \frac{\tau_{af}}{\tau_c} - \frac{\tau_{af}}{\tau_c} = 1 \quad (3-47)$$

which is contradictory to our analytical and, as we shall show soon, numerical results for black rods in a transparent medium. Even if we were to modify the Levine and Dancoff factors slightly according to some of the many prescriptions presented in the literature, the results remain equally unsatisfactory.

Thus the issue is clearly put: a profound disparity exists between the flux ratios predicted using the conventional Dancoff factor approach carried over from thermal reactor physics and our expectations based upon some rather straightforward analyses for limiting cases close to conditions of interest for FBR unit cells. This leads us directly to the subject of the next section: verification of the flux ratio function.

3.7 Numerical Verification of Flux Ratio Calculations in the Unit Cell

In this section the expressions derived in previous sections will be compared with numerical calculations of the flux ratio in a unit cell. The unit cell fluxes were calculated using Monte Carlo methods as well as S_8 transport methods.

3.7.1 Monte Carlo Unit Cell Calculations

A simple in-house Monte Carlo code, MOFLUX, was developed to calculate the fluxes in a unit cell (D3). Square unit cells and hexagonal unit cells are considered in MOFLUX, and the flux ratio is computed for various values of the optical thickness of the fuel and the coolant, and a range of source ratios. Table 3.1 summarizes the major features of this program. A limited number of calculations were also done with another Monte Carlo code, ANDY (D4), which yielded similar confirmatory results. We will present the MOFLUX results and compare them with the semi-empirical expression, Eq (3-38).

Dependence of Flux Ratio on Source Distribution. The dependence of the flux ratio on the distribution of neutron sources between the fuel and coolant was examined with the MOFLUX and ANDY codes for square and hexagonal unit cells. Both calculations yielded a similar dependence, and the results of the MOFLUX runs are presented in Fig 3.2 for three cases and compared with Eq (3-38). The numerical and analytical results agree well within $\pm 5\%$.

Dependence of Flux Ratio on Optical Thickness. The dependence of the flux ratio on fuel optical thickness was examined for square and hexagonal unit cells. As can be seen in Figure 3.3, the flux ratio calculated with MOFLUX and from Eq (3-38) are in good agreement.

Table 3.1

Major Features of the MOFLUX Code

1. Treats two region square and hexagonal cells containing a cylindrical central region.
2. Uniformly distributed neutron sources are considered for each region, covering the limits of all sources in coolant to all sources in fuel.
3. Isotropic scattering is permitted in the laboratory system (hence scattering sources are not uniformly distributed, but are proportional to the local neutron flux).
4. Neutrons penetrating the outer cell boundary are returned to the parent cell at an equivalent position.
5. A straightforward mechanistic simulation is employed — no fancy methodology is used.
6. Typical runs involve 10^4 neutron histories and comparison of repeat runs using a different initiator for the random number generator (the IBM subroutine RANNO) typically indicate a $\pm \sigma$ for the flux ratio of $\approx 6\%$.
7. Two methods are used to calculate fluxes: total path length summation and number of total events.

Figure 3.2 Effect of Source Fraction on Flux Ratio

Figure 3.3 Flux Ratio for Large Optical Thickness

Furthermore, when the flux ratio for intermediate optical thickness was examined, as in Figure 3.4, it can be seen that the slope of the flux ratio versus optical thickness curve varies between $1/3$ and $2/3$, justifying our semi-empirical formula. (Note that reciprocity permits us to reverse the role of fuel and coolant, so we do not have to consider coolant effects separately.)

These particular calculations were done for a unit cell with all sources in the coolant. In order to examine the effects of coolant optical thickness on the flux ratio more MOFLUX runs were made where only the coolant optical thickness varied. As seen in Figure 3.5, the flux ratio was insensitive to variation in coolant optical thickness when $Q_f = 0$, as predicted by Eq (3-34) and the development which precedes it.

The dependence of flux ratio on fuel scattering and the size (radius) of the fuel region was also examined. As seen in Figure 3.6, changes in fuel scattering optical thickness have very little effect on the flux ratio. This result helps justify our neglect of scattering without removal. Also, the size of the fuel lump at constant optical thickness has almost no effect on the flux ratio as seen in Figure 3.7. This confirms the expectation that optical thickness is the only geometric factor necessary to characterize the fuel rods.

Figure 3.4 Flux Ratio for Intermediate Optical Thickness

Figure 3.5 Effect of Coolant Scattering on Flux Ratio

Figure 3.6 Effect of Fuel Scattering on Flux Ratio

Figure 3.7 The Effect of Fuel Size on Flux Ratio at Constant Optical Thickness

3.7.2 S_N Transport Unit Cell Calculations

The dependence of the flux ratio on optical thickness and source distribution was also examined with S₈ transport calculations using the ANISN program (A2). The unit cell was cylindricized and white boundary conditions were used. All the previously presented cases were examined. The flux ratio versus source ratio or optical thickness curves were similar in shape to the Monte Carlo results presented in Section 3.7.1, but the absolute values were different because of the previously mentioned effects of boundary conditions involved in cell cylindricalization.

3.8 Conclusion

In this chapter it has been shown that, in order to calculate cross sections for a heterogeneous unit cell, the ratio of volume averaged coolant flux to volume averaged fuel flux (or something equivalent) must be used. Starting from the integral form of the transport equation a fairly general form for the flux ratio has been found and reduced to a special case applicable to FBR unit cells. It has been shown that this special form reproduces certain limiting cases, and agrees well with the results of Monte Carlo calculations, whereas the flux ratio calculated using the conventional IRA-NRA approach and Dancoff factors fails to reproduce these limits. Thus we are encouraged to proceed further using our flux ratio method.

CHAPTER 4

HETEROGENEOUS SELF-SHIELDING

In the previous chapter the equation defining the heterogeneous effective group cross section was derived to emphasize the need for knowledge of the ratio of coolant (including homogenized clad) to fuel fluxes, and we then proceeded to develop a simple relation for this flux ratio. In this chapter the flux ratio and the cross section equation will be combined to calculate the effects of heterogeneity on self-shielding (f factors). A new equivalence theorem will be developed for this purpose. Several applications will be discussed, with a major emphasis on blanket breeding performance.

4.1 Flux Ratio Approach to Self-Shielding

The effective group cross section for a heterogeneous medium was derived in the preceding chapter. It was shown that introducing heterogeneity into the cross section expression merely involved weighting the coolant removal term by the flux ratio, R .

Further, it was shown and verified that the flux ratio can be approximated by a simple functional relation under conditions applicable to FBR unit cells. In this section, use of this simple form of the flux ratio (Eq (3-38)) will be made to determine the effects of heterogeneity on the self-shielding (f factors).

The effective group cross section for the capture process for a heterogeneous medium with resonance absorber in the fuel region is

$$\Sigma_{\text{het}} = (\Delta u)^{-1} \int_{-\infty}^{\infty} \frac{\sum_p \sum_{c_f} (u)}{\sum_{R_f} (u) + \sum_{R_f}^n + \frac{V_c}{V_f} \sum_{R_c} R(u, Q)} du \quad (4-1)$$

$$\text{where } \sum_p = \sum_{s_f}^n + \sum_{sc} + \sum_{pa} \quad (4-2)$$

$$\sum_{R_c} = \sum_{sc} + \sum_{ac} \quad (4-3)$$

$$\left. \begin{array}{l} \sum_{c_f} (u) \\ \sum_{R_f} (u) \end{array} \right\} \begin{array}{l} \text{are the resonance capture and removal} \\ \text{cross sections of the resonance} \\ \text{absorber in the fuel pin} \end{array}$$

$\sum_{pa}$ is the potential scattering cross section of the resonance absorber in the fuel pin

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$$\left. \begin{array}{l} \sum^n s_f \\ \sum^n R_f \end{array} \right\} \text{ are the non-resonant scattering and removal cross sections of the non-resonant elements in the fuel pin}$$

$$\left. \begin{array}{l} \sum_{ac} \\ \sum_{sc} \end{array} \right\} \text{ are the capture and scattering cross sections of the coolant}$$

In the narrow resonance approximation used here, "removal" occurs in both scattering and absorption reactions for both media.

The flux ratio is, in our approximate prescription,

$$R(u, Q) = \frac{1 + \omega \tau_f(u) Q_c}{1 + \frac{1}{3} \tau_c Q_f} \quad (4-4)$$

or, to simplify the relation in what follows:

$$R(u, Q) = \eta (1 + \alpha \Sigma_{R_f}(u)) \quad (4-5)$$

$$\text{where } \eta = (1 + \frac{1}{3} \tau_c Q_f)^{-1} \quad (4-6)$$

$$\alpha = \omega \bar{\ell}_f Q_c \Sigma_r \quad (4-7)$$

$\tau_f(u)$ is the total optical thickness of the resonance absorber in the fuel pin

τ_c is the total optical thickness of the coolant

$\bar{l}_f$ is the Dirac chord length through the fuel pin, and $1/3 \leq \omega \leq 2/3$, depending on the optical thickness of the fuel; in what follows we will anticipate the numerical results of subsequent sections and take $\omega \equiv 1/3$, the applicable lower limit.

Using the single level Breit-Wigner formula for the resonance cross section, Eq (4-1) can be normalized and simplified; from this point onwards, we limit consideration to a single isolated resonance:

$$\bar{\sigma}_{het} = \frac{\sigma_r \Gamma \gamma}{2E_r \Delta u} \int_{-\infty}^{\infty} \frac{(\beta + \bar{\beta}) \psi(x, t)}{\psi(x, t) + \phi \chi(x, t) + \bar{\beta} + \beta R(x, Q)} dx \quad (4-8)$$

where σ_r is the total resonance cross section at resonance energy E_r

$$\beta = \frac{N_c}{N_o} \frac{V_c}{V_f} \frac{\sigma_{Rc}}{\sigma_r} \quad (4-9)$$

$$\bar{\beta} = \frac{\sigma_{pa}}{\sigma_r} + \frac{N_f}{N_o} \frac{\sigma_{Rf}^n}{\sigma_r} \quad (4-10)$$

and the other parameters such as x , t , Γ_γ , Δu , and ϕ are defined in section 2.2.

Inserting the single level Breit-Wigner resonance cross section formulas into the expression for $R(x,Q)$, Eq (4-5), and then inserting this new expression into Eq (4-8), gives:

$$\bar{\sigma}_{het} = \frac{\sigma_r \Gamma_\gamma}{2E_r \Delta u} \int_{-\infty}^{\infty} \frac{(\beta + \bar{\beta}) \psi(x,t)}{[1 + \delta] [\psi(x,t) + \phi \chi(x,t) + \bar{\beta} + \beta \frac{\eta}{1 + \delta}]} dx \quad (4-11)$$

$$\text{where } \delta = \alpha \beta \eta \quad (4-12)$$

Equation (4-11) can be written in an even more compact form by defining

$$B = \bar{\beta} + \beta \quad (4-13)$$

and

$$B' = \bar{\beta} + \beta \frac{\eta}{1 + \delta} \quad (4-14)$$

Then the heterogeneous effective group cross section is given by:

$$\bar{\sigma}_{\text{het}} = \frac{\sigma_r \Gamma \gamma}{2E_r \Delta u} \frac{B/B'}{1+\delta} \int_{-\infty}^{\infty} \frac{B' \psi(x,t)}{\psi(x,t) + \phi \chi(x,t) + B'} dx \quad (4-15)$$

The homogeneous cross section can be obtained from Eq (4-1) by setting $R(u,Q) \equiv 1$ (or $\eta = 1$ and $\alpha = 0$) in Eq (4-11). When this limiting case is examined it can be seen that the integrand of the cross section expression has the same mathematical form as the integrand in Eq (4-15), the only difference being that B' is replaced by B . Therefore the heterogeneous effective group cross section (and consequently the self-shielding f factor) can be expressed in terms of a homogeneous effective group cross section (or the corresponding homogeneous self-shielding f factor). We will deal exclusively with f factors from this point onward; the self-shielding f factor for the capture process in the resonance under consideration is then:

$$f_{\text{het}}(B) = \frac{B/B'}{\pi(1+\delta)} \int_{-\infty}^{\infty} \frac{B' \psi(x,t)}{\psi(x,t) + \phi \chi(x,t) + B'} dx \quad (4-16)$$

or

$$f_{\text{het}}(B) = \frac{B/B'}{\pi(1 + \delta)} f_{\text{hom}}(B') \quad (4-17)$$

Finally, the relationship between the heterogeneous and homogeneous self-shielding f factor can be obtained from Eq (4-17)

$$\frac{f_{\text{het}}(B)}{f_{\text{hom}}(B)} = \frac{B/B'}{1 + \delta} \cdot \frac{f_{\text{hom}}(B')}{f_{\text{hom}}(B)} \quad (4-18)$$

The relation between the heterogeneous and homogeneous self-shielding factors, given by Eq (4-18), is a new equivalence relation. This relation permits the calculation of heterogeneous self-shielding factors in terms of homogeneous self-shielding factors for a given unit cell.

Although we have considered the case of a single resonance here, Eq (4-18) may be applied to a coarse group of a multigroup set by either considering a "representative" resonance from that group or by using an expanded version of this relation, derived by summing over all resonances in the group. We will see shortly that

this added sophistication is not needed, because of the weak variation of $f_{\text{het}}/f_{\text{hom}}$ with neutron energy.

The equivalence relation given by Eq (4-18) can also be approximated analytically. From Eqs (4-12), (4-13), and (4-14), the first part of the right hand side of Eq (4-18) becomes:

$$\frac{B/B'}{1 + \delta} = \frac{1}{1 + \delta \left(1 - \frac{\beta/B}{Q_c} \right)} \quad (4-19)$$

Before examining the remainder of the right hand side of Eq (4-18), it is useful to calculate how much B changes due to heterogeneity:

$$\Delta B = B' - B = - \frac{\delta \beta}{1 + \delta Q_c} \quad (4-20)$$

In order to calculate the fractional change in B , one divides both sides of Eq (4-20) by B to obtain:

$$\frac{\Delta B}{B} = - \frac{\delta \beta/B}{1 + \delta Q_c} \quad (4-21)$$

Note that the same factor, $\frac{\beta/B}{Q_c}$, appears in both Eq (4-19) and Eq (4-21). This factor, for most FBR unit cell geometries and compositions, is of the order of 0.5, and in some cases can exceed unity slightly. As we will see later, δ , which is a function of τ_c , the coolant optical thickness, is on the order of 0.1. From these representative values for a FBR unit cell, it can be seen that the introduction of heterogeneity typically changes B by several per cent, and always less than 10 %.

Since B changes by only a few per cent, the resulting change in the homogeneous self-shielding factor can be calculated by expanding $f_{\text{hom}}(B')$ in a Taylor series around B , and neglecting higher order terms:

$$f_{\text{hom}}(B') = f_{\text{hom}}(B) + \frac{df_{\text{hom}}(B)}{d\beta} \Delta\beta + \dots \quad (4-22)$$

In Eq (4-22), the fact that the changes in B stem from changes in β and not $\bar{\beta}$ is used: introduction of heterogeneity modifies only the coolant part of the non-resonant parameters; the non-resonant parameters of the fuel pin are unaffected. Therefore, $\Delta\beta$ is also calculated by Eq (4-20):

$$\frac{\Delta\beta}{\beta} = - \frac{\delta}{1 + \delta} \frac{1}{Q_c} \quad (4-23)$$

The variation of the self-shielding factor with β can be estimated using the approximate expression for f given in Eq (2-31), which is reproduced here in current notation:

$$f_{\text{hom}}(B) = \left[\frac{\bar{\beta} + \beta}{\bar{\beta} + \beta + 1} \right]^{1/2} \quad (4-24)$$

from which

$$\frac{df_{\text{hom}}(B)}{d\beta} = \frac{1}{2} f_{\text{hom}}^{-1}(B) (1 - f_{\text{hom}}^2(B)) \quad (4-25)$$

Define

$$\gamma(B) = \frac{d[\ln f_{\text{hom}}(B)]}{d[\ln B]} = \beta f_{\text{hom}}^{-1}(B) \frac{df_{\text{hom}}(B)}{d\beta} \quad (4-26)$$

then

$$\frac{f_{\text{hom}}(B')}{f_{\text{hom}}(B)} = 1 + \gamma(B) \frac{\Delta\beta}{\beta} \quad (4-27)$$

Inserting Eqs (4-24), (4-25), and (4-26) into Eq (4-27), one gets:

$$\frac{f_{\text{hom}}(B')}{f_{\text{hom}}(B)} = 1 - \frac{1}{2}(1 - f_{\text{hom}}^2(B)) \cdot \frac{\beta/B}{Q_c} \cdot \frac{\delta}{1 + \delta} \quad (4-28)$$

Now all the expressions required to evaluate Eq (4-18) are available.

Inserting Eqs (4-19), (4-28) into Eq (4-18) yields

$$\frac{f_{\text{het}}(B)}{f_{\text{hom}}(B)} = \frac{1}{1 + \delta \left(1 - \frac{\beta/B}{Q_c} \right)} \cdot \left[1 - \frac{1}{2}(1 - f_{\text{hom}}^2(B)) \frac{\delta}{1 + \delta} \frac{\beta/B}{Q_c} \right] \quad (4-29)$$

Considering that the second term in the denominator and the second term inside the parenthesis on the right hand side of Eq (4-29) are both much less than 1.0 , one can further simplify the equation:

$$\frac{f_{\text{het}}(B)}{f_{\text{hom}}(B)} \approx 1 - \delta \left[1 - \left(1 - \frac{1 - f_{\text{hom}}^2(B)}{2(1 + \delta)} \right) \right] \frac{\beta/B}{Q_c} \quad (4-30)$$

In deriving Eqs (4-29) and (4-30), several new parameters were introduced for convenience. It is more meaningful to express the final approximate equivalence relation in terms of the optical thickness of the coolant and the source fraction:

$$\frac{f_{\text{het}}(\sigma_0)}{f_{\text{hom}}(\sigma_0)} \approx 1 - \frac{1}{3} \tau_c Q_c \left[1 - \frac{1 + f_{\text{hom}}^2(\sigma_0) Q_c^*}{2 Q_c} \right] \quad (4-31)$$

where Q_c^* is defined as

$$Q_c^* = \frac{\beta}{B} = \frac{\sigma_0}{\sigma_0 + \sigma_{p_a}} \quad (4-32)$$

In section 4.2 we will see that this "source ratio" has a special significance. Equation (4-31) relates the heterogeneous and homogeneous self-shielding factors in terms of the coolant properties. Through use of this equation, given the homogeneous self-shielding factor and the geometry and the composition of the unit cell, one can calculate the heterogeneous self-shielding factor. For a unit cell with $Q_c \approx Q_c^*$, Eq (4-31) simplifies to

$$\frac{f_{\text{het}}(\sigma_0)}{f_{\text{hom}}(\sigma_0)} \approx 1 - \frac{1}{6} (1 - f_{\text{hom}}^2(\sigma_0)) \tau_c Q_c \quad (4-33)$$

which approaches the correct limit of 1.0 for unshielded or lightly-shielded groups, where $f_{\text{hom}} \rightarrow 1.0$.

When Eq (4-31) is examined further, it can be seen that for a unit cell with $Q_c^* \neq Q_c$, the correct limit for lightly shielded groups cannot be obtained. For an infinitely dilute case, $\sigma_0 = \infty$, $f = 1$), the equation reduces to:

$$\frac{f_{\text{het}}(\sigma_0)}{f_{\text{hom}}(\sigma_0)} = 1 - \frac{1}{3} \tau_c (Q_c - Q_c^*) \quad (4-34)$$

which is physically unrealistic.

This short-coming of Eq (4-31) is due to the form of $R(x,Q)$ chosen in the early steps of the approximation. When Eq (4-4) is examined, it can be seen that far away from the resonance peak, $R(x,Q)$ has a value of:

$$R(\infty,Q) = \frac{1 + \frac{1}{3} \bar{\ell}_f N_c \sigma_p Q_c}{1 + \frac{1}{3} \tau_c Q_f} \quad (4-35)$$

which may not be equal to unity.

In the usual approach to resonance region analysis, it is assumed that the flux recovers to its asymptotic spatially uniform value far away from the resonance peak energy. When Eq (4-35) is not equal to unity, the method used here contradicts this flat flux approximation: it predicts a difference between fuel and coolant fluxes even at energies far away from the resonance energy.

In order to be consistent with the flat flux approximation, we consider Eq (4-8) and replace $R(x,Q)$ by a normalized $R'(x,Q)$ where

$$R'(x,Q) = \frac{R(x,Q)}{R(\infty,Q)} \quad (4-36)$$

which, for small values of the optical thickness, can be written

$$R'(x, Q) \approx 1 + \frac{1}{3} \tau_{fr} Q_c \quad (4-37)$$

where

$$\tau_{fr} = \bar{\chi}_{f o r} N \sigma (\psi(x, t) + \phi \chi(x, t)) \quad (4-38)$$

Note that this renormalization merely amounts to replacing the region optical thickness by the region optical thickness minus its asymptotic value: an expedient which has almost no effect on the value of R near the resonance, but which forces R to approach unity at the wings. Inserting Eq (4-37) into Eq (4-8), and after rearranging the terms, one gets:

$$f_{het}(B) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\tilde{B} \psi(x, t)}{\psi(x, t) + \phi \chi(x, t) + \tilde{B}} dx \quad (4-39)$$

$$\text{where } \tilde{B} = \frac{\beta + \bar{\beta}}{1 + \frac{1}{3} \tau_{fr} Q_c} \quad (4-40)$$

Eq. (4-39) can be simplified to:

$$\frac{f_{\text{het}}(B)}{f_{\text{hom}}(B)} = \frac{f_{\text{hom}}(\tilde{B})}{f_{\text{hom}}(B)} \quad (4-41)$$

and $f_{\text{hom}}(\tilde{B})$ can be calculated by expanding it in a Taylor series around B . (As can be seen from Eq (4-40), $\tilde{B}$ is only a few per cent different from the homogeneous value B .) Then Eq (4-41) becomes

$$\frac{f_{\text{het}}(\sigma_0)}{f_{\text{hom}}(\sigma_0)} = 1 - \frac{1}{2}(1 - f_{\text{hom}}^2(\sigma_0)) \frac{\frac{1}{3} \tau_c Q_c}{1 + \frac{1}{3} \tau_c Q_c} \quad (4-42)$$

or, neglecting second order terms:

$$\frac{f_{\text{het}}(\sigma_0)}{f_{\text{hom}}(\sigma_0)} = 1 - \frac{1}{6}(1 - f_{\text{hom}}^2(\sigma_0)) \tau_c Q_c \quad (4-43)$$

which is identical to Eq (4-33): i.e., the same result could have been achieved by source renormalization in Eq (4-31). Eq (4-43) reproduces the correct limit of 1.0 when $f_{\text{hom}}(\sigma_0)$ approaches unity.

The use of the un-normalized $R(x,Q)$ in numerical calculations introduces an error which usually slightly overestimates the effects of heterogeneity. The effect of normalization on the integrand of the self-shielding factor, f , is illustrated in Fig 4.1. The difference between the integrands of the homogeneous and heterogeneous f factors, ΔI , is plotted versus the reduced energy, x , for the 102.6 eV resonance of U-238. As seen in Fig 4.1, ΔI , using the un-normalized $R(x,Q)$, is larger in the wings of the resonance than when the normalized $R(x,Q)$ is used. Also note that when the two limiting slopes of $R(x,Q)$ are compared to the "exact" case, it is seen that the slope of $1/3$ is the best choice — confirming our previous assumption. Similar calculations for the 6.67 eV resonance give plots similar in all important respects to that for the 102.6 eV resonance.

In section 4.3 the relation between the heterogeneous and homogeneous self-shielding factors will be examined for metal and oxide fueled unit cells, by comparing the results of the intermediate form (Eq (4-31)), the final approximation (Eq (4-43)), and numerical (CIDI code) calculations.

Figure 4.1 The Effect of Flux Ratio Slope on the Heterogeneous Integrand

However, first we must address the long-postponed question of how to compute the source fraction, Q_c .

4.2 The Source Fractions Q_c and Q_f

We have previously referred to the need for region-wise source fractions, but did not discuss how they were to be obtained. The source fractions were defined by Eqs (3-16) and (3-17), namely:

$$Q_f = \frac{S_f V_f}{S_f V_f + S_c V_c} \quad (4-44)$$

$$Q_c = \frac{S_c V_c}{S_f V_f + S_c V_c} \quad (4-45)$$

where S_f and S_c are the number of neutrons per unit volume "produced" (here, by moderation) in the fuel and coolant-clad regions, respectively.

As discussed in section 2.1, the neutron flux in the absence of a resonance is considered to be the same throughout the cell. Therefore, the number of neutrons per unit volume of the

region under consideration slowing down into the resonance energy group is:

$$S_{\alpha} = \xi_{\alpha} \sum_s \bar{\phi}_0 \quad (4-46)$$

where α stands for f (fuel) or c (coolant-clad)

$\bar{\phi}_0$ is the unperturbed cell flux

ξ_{α} is the average lethargy gain per scattering collision

Using Eq (4-46) in Eqs (4-44) and (4-45), it follows that

$$Q_f = \frac{\xi_f \sum_{sf} V_f}{\xi_f \sum_{sf} V_f + \xi_c \sum_{sc} V_c} \quad (4-47)$$

$$Q_c = \frac{\xi_c \sum_{sc} V_c}{\xi_f \sum_{sf} V_f + \xi_c \sum_{sc} V_c} \quad (4-48)$$

or, in more compact form,

$$Q_c = (1 + H)^{-1} \quad (4-49)$$

$$Q_f = 1 - Q_c \quad (4-50)$$

$$\text{where } H = \frac{\xi_c v_c \sum_{sc}}{\xi_f v_f \sum_{sf}} \quad (4-51)$$

$\sum_{sf}$ includes the scattering cross section of the non-resonant element in the fuel pin as well as the potential scattering of the resonance absorber.

The lethargy gain parameter, ξ_α , should, in theory, account for both elastic and inelastic moderation. However, as shown in Fig 4.2, the elastic moderation source dominates in the region of current interest, even in a fast reactor (D5). Thus

$$\xi \approx \xi_{\text{elastic}} \approx \frac{2}{A + \frac{2}{3}} \quad (4-52)$$

Equations (4-49) through (4-52) were used to evaluate source ratios in the analytical and numerical computations discussed in the

Figure 4.2 Source Contributions in Fast Reactor Core

remainder of this chapter. However, in something of an aside, we might also at this point note the alternative form for Eq (4-48):

$$Q_c = \frac{\xi_c \tau_c}{\xi_f \tau_{fo} + \xi_c \tau_c} \quad (4-53)$$

where $\left. \begin{array}{l} \tau_c \\ \tau_{fo} \end{array} \right\}$ are the non-resonant optical thicknesses of the coolant and the fuel pin, respectively

This presentation suggests further discussion of the apparent inconsistency in the concurrent use of the NR formulation and Eq (4-4) for the flux ratio R .

Note that for R to approach 1.0 asymptotically in the wings of the resonance, we would have to have (instead of Eq (4-53), which is actually used) a source fraction defined as:

$$Q_c^* = \frac{\tau_c}{\tau_c + \tau_{fo}} \quad (4-54)$$

When both fuel and coolant contain moderator ($\xi_c \approx \xi_f$), the difference between the source ratio Q_c and Q_c^* is not appreciable; however, for metal fuel, where $\xi_f \approx 0$, the discrepancy is quite evident. Also note that Eq (4-54) is merely another form of Eq (4-32), which appeared as the natural consequence of the derivation leading to Eq (4-31). As we saw in the preceding section, this difference in source ratios, Eq (4-53) versus Eq (4-54), must be resolved if R is to approach unity in the region far removed from the peak of the resonance. The method chosen was to replace τ by $(\tau - \tau_{\text{asymptotic}})$ in R , since this gives correct limits both near to and far from the peak of the resonance.

4.3 Effects of Heterogeneity on Self-Shielding f Factors for LMFBR Blankets

In the previous section, the effect of heterogeneity on self-shielding factors was examined. In this section, a case study for two FBR Blanket unit cells will be made to determine the best slope, ω , in the flux ratio relation, and to test the approximate expressions given in the previous section.

In order to examine the general behavior of self-shielding factors, three artificial energy groups, each containing only one resonance, were considered. The resonances were chosen such that they are representative of the majority of the resonances at low, intermediate, and high energies. The three representative resonances

are the 6.67 eV , 102.6 eV , and 1054 eV resonances of U-238; and the energy group structure of the three groups is shown in Table 4.1.

4.3.1 Self-Shielding for UO₂ Fueled Blanket Unit Cells

The UO₂ fueled blanket unit cell considered here is from a hexagonal lattice as shown in Fig 3.1. The composition and the dimensions of the unit cell are identical to those of the blanket oxide/sodium subassembly constructed for use in the Blanket Test Facility (BTF) at MIT (L5, D6). The homogenized atom densities of the Blanket Mock-up No. 4 are very similar to a standard FBR Blanket's homogenized atom densities: most mock-up assemblies are uranium metal fueled, but the oxide/sodium assembly is a physically realistic reproduction of a real reactor's radial blanket fuel. We should also note that heterogeneity in the radial blanket is in some respects more severe than in an LMFBR core, due to the larger diameter fuel rods and softer spectrum; it is considerably larger than in a Gas Cooled Fast Reactor where the coolant is essentially transparent. Thus the results discussed here deal with an example for which heterogeneous effects are accentuated: only in thick-plate-type critical assemblies are larger effects to be expected.

The self-shielded resonance capture cross section of the three above-mentioned representative energy groups were calculated using the CIDI code. In order to determine the best slope of the

Table 4.1

The Energy Group Structure of the Three
Representative Energy Groups

Group	Upper Energy (eV)	Lower Energy (eV)	Resonance Energy (eV)
1	1100	1000	1054
2	150	80	102.6
3	12	2	6.67

flux ratio, ω , three different values of ω were considered: ω was successively taken to be $1/3$ or $2/3$ (the limiting values) and the results were then compared with the case when ω is represented by an "exact" expression fitted to the Monte Carlo results presented in Chapter 3. The results are presented in Table 4.2. All results except those of Eq (4-31) are based upon use of a normalized source ratio, $R'(x,Q)$.

Examining Table 4.2, it can be seen that the slope of $\omega = 1/3$ is a relatively good approximation to the exact case. Also, the ratio of heterogeneous to homogeneous factors is approximately the same for all three groups — this is particularly true for the approximate equations. This is due to the fact that once the slope, ω , is set, all the parameters in Eqs (4-31) and (4-43) depend almost entirely on the coolant properties, and in these calculations we have considered a coolant with parameters independent of the group energies. Thus one gets almost equal heterogeneous effects in each group, and the small difference in self-shielding factors is due to the term in Eqs (4-31) and (4-43) which contains the f factor, which varies from group to group. The higher the energy of the group or the more dilute the system, the closer f is to 1.0, and thus the net effect due to this term diminishes. As seen in Table 4.2, the approximation that does not use the normalized flux ratio, R' , underestimates the heterogeneity effect. In any event, the heterogeneous effect in an oxide cell

Table 4.2

Effects of Heterogeneity on U-238 Capture Self-Shielding Factor

for Three Energy Groups for a UO₂ Fueled Unit Cell:

(All Data Calculated Using CIDI Program)

$$\text{Ratio} = \frac{f_{\text{het}}}{f_{\text{hom}}}$$

Group	Homogeneous f_c	ω			Approximate Values	
		1/3	"exact"	2/3	Eq (4-31)	Eq (4-43)
1	0.198	0.989	0.986	0.974	0.9906	0.9902
2	0.0437	0.992	0.987	0.979	0.9902	0.9898
3	0.0386	0.992	0.987	0.978	0.9902	0.9898

is very small indeed: much less than the $\pm 10\%$ uncertainty currently assigned to U-238 capture cross-section values. The small resonance-to-resonance and group-to-group variation in the heterogeneity correction also justifies dealing with a single representative resonance in the preceding analyses instead of the more correct summations over all resonances in a group.

4.3.2 Self-Shielding Factor for U-Metal-Fueled Blanket Unit Cells

The metal-fueled blanket unit cell considered here is from a square lattice, as shown in Fig 3.1. Like the oxide-fueled unit cell, this unit cell has a homogeneous composition identical to that of the blanket subassemblies used in the BTF at MIT (L5, D6); further, the unit cell dimensions are those of the uranium fueled, steel clad, sodium chromate "moderated" standard BTF blanket assemblies.

Calculations similar to those of section 4.3.1 were made for this metal-fueled unit cell and the results are given in Table 4.3. It is seen that the best slope, ω , is again $1/3$ as observed in the previous section. The effect of heterogeneity is more apparent here due to the small value of Q_f . Since most of the sources are concentrated in the coolant region, the effect of fuel-lumping is larger than that of oxide fuel, which generates an appreciable internal slowing-down source.

Table 4.3

Effects of Heterogeneity on U-238 Capture Self-Shielding Factor
 for Three Energy Groups for a Metal-U-Fueled Unit Cell
 (All Data Calculated Using CIDI Program)

$$\text{Ratio} = \frac{f_{\text{het}}}{f_{\text{hom}}}$$

Group	Homogeneous f_c	ω			Approximate Values	
		1/3	"exact"	2/3	Eq (4-31)	Eq (4-43)
1	0.198	0.976	0.973	0.953	0.9796	0.9833
2	0.0437	0.977	0.972	0.959	0.9791	0.9827
3	0.0386	0.979	0.972	0.958	0.9791	0.9827

Again, use of the limiting slope of $1/3$, and the approximate equivalence relations is justified, although here it is not clear that normalization of R was of any particular benefit.

The effects of heterogeneity on the self-shielding factor have now been determined for oxide and metal unit cells. We must next examine the resulting changes in a key integral property of the blanket — the breeding ratio.

4.4 Effects of Changes in Self-Shielding Factors on Blanket Breeding Ratio

In the preceding section, the changes in f factor due to heterogeneity were examined. In this section, the effect of such changes on FBR breeding ratios will be examined.

In order to bracket the problem, a much larger variation in self-shielding factors will be considered. The self-shielding will be varied from no shielding ($\sigma_0 = \infty$) to a totally-shielded ($\sigma_0 = 0$) case. While the variation is physically unrealistic, some very interesting insights can be gained by permitting this wide variation.

Consider a cylindrical FBR with two core enrichment zones and three rows of radial blanket assemblies. The size of the core and blanket and the concentration of the various constituent isotopes are taken similar to the ZPPR-2 (hence a CRBR demonstration-size reactor) core and blankets (W2, T2). Using a homogeneous

one-dimensional (radial) model for this system, the capture rates were calculated using ANISN S_8 26-group calculations for a series of computations in which only the U-238 shielding factors were changed. Properties were kept unchanged in one region (e.g., core) while being varied in the other region (blanket). The changes in self-shielding were introduced by using successive sets of f values corresponding to tabulated values of σ_0 . The results are presented in Tables 4.4 and 4.5.

As seen in Table 4.4, the radial blanket breeding ratio changes by less than 20 % when U-238 self-shielding changes from none to total. Considering the much smaller changes in σ_0 due to heterogeneity (typically, the σ_0 of ~ 25 barns is decreased by the equivalent of ~ 0.8 b in terms of the net effect on f), the changes in the breeding ratio of the radial blanket due to blanket heterogeneity will not be appreciable (less than a fraction of one per cent). The breeding ratio and the multiplication constant of the core (Table 4.5) are considerably more sensitive to self-shielding, but even here the incremental effects of heterogeneity can not be appreciable. In the core, however, the effect on reactivity, where fractions of a per cent differential are of interest, is of paramount concern. In this regard, it was found that changes in blanket shielding did not affect the system multiplication constant appreciably, as shown in Table 4.5. A more detailed discussion of an even more extensive parametric analysis of the effect of

Table 4.4

Radial Blanket Breeding Ratio as a Function of U-238 Self-Shielding
in the Blanket for Two Different Degrees of Shielding in the Core

σ_0 in the Blanket	Radial Blanket Breeding Ratio			
	for Core	System	for Core	System
	$\sigma_0 = 0$	k	$\sigma_0 = 100$	k
∞	0.26	1.138	0.28	1.085
10^4	0.26	1.138	0.28	1.085
10^3	0.26	1.139	0.28	1.086
10^2	0.25	1.141	0.28	1.086
10^1	0.23	1.144	0.25	1.101
0	0.22	1.146	0.24	1.103

Table 4.5

Changes in Core Breeding Ratio as Core Self-Shielding is Varied,
for Infinitely Dilute Blanket Cross Sections

σ_0 in the Core	Core Breeding Ratio for Blanket $\sigma_0 = \infty$	System k
∞	0.77	1.053
10^4	0.77	1.062
10^3	0.74	1.072
10^2	0.67	1.093
10^1	0.57	1.125
0	0.53	1.138

self-shielding on breeding ratio can be found in Ref (W3).

4.5 Observations and Conclusion

In this chapter a new equivalence theorem for calculation of the effects of heterogeneity in FBR lattices has been derived. In addition, a simple analytic approximation has been developed from the more general relation. The approximate relation shows in an explicit way the effect of moderation in the fuel, which acts to decrease heterogeneous effects, and which is easily overlooked if one applies thermal reactor treatments based on a dominant coolant-moderator source.

The analytical results were applied to a typical case involving a FBR blanket, and to blanket mock-up assemblies used at MIT. Several important results were developed:

- (a) The effects of blanket heterogeneity are shown to be quite small, and negligible with respect to prediction of breeding performance.
- (b) The metal and oxide-fueled assemblies have appreciably different heterogeneity increments in their effective cross sections, but fortunately, as noted in (a) above, these are no practical consequences of concern.

It is interesting to note that the original design of the MIT blanket mock-up fuel assemblies was based on matching the optical absorption thickness of its metal fuel to that of the UO_2 fuel rods used in a real reactor. As we have discovered in the present work, this reasoning is invalidated by the effect of the appreciable slowing-down source provided by the oxygen in the UO_2 , which is absent in the metal.

Finally, although the various equations were derived for the capture reaction, the same expressions hold for the self-shielding factors for scattering. In Eq (4-43), for example, one merely employs the f_{hom} values appropriate to scattering — since scattering interaction f values are generally quite close to unity, the heterogeneous correction is even smaller than that for the capture reaction.

CHAPTER 5

SUMMARY, CONCLUSION, AND RECOMMENDATIONS

In this chapter we will summarize the work reported here, and draw conclusions. Some suggestions on further research in this area will also be presented.

5.1 Summary5.1.1 Introduction

The objective of the work reported here was to carry out a detailed examination of the effects of heterogeneity on resonance self-shielding in fast reactor applications with particular emphasis on the blanket region and on its dominant reaction - capture in U-238. The results, however, are more general, and apply equally well to scattering resonances, to other isotopes (fertile, fissile and structural species) and to other reactor environments, so long as the underlying assumptions apply (basically those of narrow resonance theory).

The approach followed in the analysis involved casting the heterogeneous resonance integral into a form involving the ratio of

coolant-to-fuel fluxes, and then developing a generalized correlation for this ratio, using both integral transport and collision probability theory to infer the form of the correlation, and then relying upon Monte Carlo calculations to verify the absolute results.

It was found that a simple linear prescription could be developed for the flux ratio as a function of fuel optical thickness and the fraction of the slowing-down source generated by the coolant. This in turn permitted casting the heterogeneous resonance integral in the form of a homogeneous integral with a modified value of the background scattering cross section per resonance absorber nucleus, σ_0 . The resulting new equivalence theorem is a major achievement of the present work. A simple version of this relation was also developed and used to show that heterogeneity effects are negligible in fast reactors.

The paragraphs which follow summarize each of the above outlined steps in the analysis.

5.1.2 Homogeneous Self-Shielding

The first step in the analysis was to review the general topic of self-shielding in homogeneous media with particular emphasis on fertile nuclei in fast reactors. Based upon this review it was concluded that the subsequent work could proceed under the following simplifying assumptions.

- (a) Absorption or scattering interactions remove neutrons from an energy group wide enough to contain only one resonance.
- (b) Neutrons are supplied by elastic or inelastic down scattering and this distributed neutron source is a smooth function of lethargy.
- (c) The unperturbed total group flux is used rather than the perturbed flux - which dips where resonance cross sections peak - the resulting error is small (eg. $\sim 0.4\%$ for U-238).
- (d) The Narrow Resonance Approximation is acceptable for almost all high energy resolved resonances. The resonances are separated such that the flux recovers from Placzek oscillations, and also the resonances do not overlap or interfere.
- (e) Furthermore, since the self-shielding effects are more pronounced at intermediate and low energies, only the resolved resonance region is considered along with the single level Breit-Wigner formula for the cross section.

Under the above assumptions broad group multigroup cross sections in the resonance region are given by:

$$\bar{\Sigma}_{xg} = \frac{\sum_{k=1}^K \int_{\Delta E} \Sigma_{xk}(E) \bar{\phi}_k(E) dE}{\int_{\Delta E} \bar{\phi}(E) dE} \quad (5-1)$$

where

$\Sigma_{xk}(E)$ is the resonance cross section for nuclear process x ,
of the k^{th} resonance in broad group g , which contains
 K resonances;

$\phi_k(E)$ is the perturbed neutron flux in the presence of the
 k^{th} resonance,

$\phi(E)$ is the unperturbed neutron flux, and

ΔE is the width of the g th energy group.

The perturbed and unperturbed fluxes in Eq. (5-1) are found to be

$$\bar{\phi}(E) = \frac{C_o (E_o/E)^n}{\Sigma_o} \quad (5-2)$$

$$\bar{\phi}_k(E) = \frac{C_o (E_o/E)^n}{\Sigma_{Rk}(E)} \quad (5-3)$$

where

E_b is the maximum energy of the coarse energy group,

C_o is a constant for each group,

Σ_o and $\Sigma_{R_k}(E)$ are the non-resonant and resonant removal cross sections of the medium, and

n is the flux shape exponent, which is usually taken to be 1.0 (1/E spectrum).

Using Eqs. (5-2) and (5-3) along with the Breit-Wigner formula for the cross sections, Eq. (5-1), for the capture process reduces to

$$\bar{\sigma}_c = \frac{\sigma_r}{\Delta u} \cdot \frac{\Gamma_Y}{2E_r} \int_{-\infty}^{\infty} \frac{\Psi(x,t)}{\Psi(x,t) + \Phi\chi(x,t) + \beta'} dx \quad (5-4)$$

where

σ_r is the Doppler broadened cross section at the peak of the resonance

Δu is the group lethargy width, (i.e. $n = 1$)

Γ_Y is the capture width

E_r is the energy at which the peak of the resonance occurs

Φ is the scattering fraction of the total resonance cross section

β is the ratio of the non-resonance removal cross section per absorber nucleus to the maximum removal cross section at the resonance peak of the resonant absorber.

$\psi(x,t)$ and $\chi(x,t)$ are the symmetrical and anti-symmetrical Voigt shape functions, respectively (D1),

where

$$x = 2 \frac{E - E_r}{\Gamma}$$

$$t = \frac{4E_r kT}{\Gamma^2}$$

and

Γ is the total resonance width.

Equation (5-4) was used as the basis for a computer program (CIDI, described in Appendix A) which carries out the required numerical integration. As a check (and for later use to calculate self-shielding factors) it was used to calculate cross sections at infinite dilution, for which an analytical result is available:

$$\sigma_{\infty} = \frac{\pi}{2} \frac{\sigma_r}{\Delta u} \frac{\Gamma}{E_r} \quad (5-5)$$

The results of the numerical calculation for the group structure used in the Bondarenko cross section set (B2), and the

analytical values, along with the values tabulated by Bondarenko for U-238 are presented in Table 5.1. As can be seen, the numerical and analytical results are in excellent agreement; Bondarenko's values, which are based on cross section data over ten years older than that used here, differ slightly.

The self shielding factor of group g for nuclear process x , f_{xg} , is defined as:

$$f_{xg} = \frac{\sigma_{xg}}{\sigma_{xg\infty}} \quad (5-6)$$

where

σ_{xg} is the self-shielded effective cross section for process x of group g

$\sigma_{xg\infty}$ is the infinite dilution cross section for process x of group g .

The self-shielded effective cross sections are calculated by changing the absorber density (hence σ_0) in the pertinent cross section formulas (i.e. Eq. (5-4) for capture).

Self-shielding f factors were then calculated for various degrees of self-shielding, which is measured by the parameter σ_0 , the total non-resonant cross section per absorber nucleus. The self-shielding factors were also calculated for

TABLE 5.1

Comparison of Infinite Dilution Capture Cross Sections of U-238

Group	Upper Energy Bound	Analytical Value Eq (5-5) (barns)	Numerical Value Eq (5-4) CIDI Program (barns)	Bondarenko Set (barns)
14	2.15 keV	1.718	1.716	2.10
15	1 keV	3.582	3.575	3.60
16	465 eV	4.617	4.608	4.50
17	215 eV	20.583	20.463	17.0
18	100 eV	16.015	15.992	15.0
19	46.5 eV	55.673	55.532	58.0
20	21.5 eV	81.020	80.747	82.0
21	10 eV	169.880	169.06	171.0
(22	4.65 eV)			

different ambient temperatures, which affect the results through the parameter t in the Voigt functions.

The general dependence of the f factor on σ_o or the temperature has not been formulated in closed analytical form. However, approximate relations between f factors and σ_o or temperature were used as a qualitative check on the functional dependence of the calculated values of the f factors. It can be shown that the dependence of f on σ_o is given by the approximate form: (S3)

$$f \approx \left| \frac{\sigma_p + \sigma_o}{\sigma_r + \sigma_p + \sigma_o} \right|^{1/2} \quad (5-7)$$

where

σ_p is the potential cross section of the resonance absorber

σ_r is the cross section at the resonance peak

Equation (5-7) suggests a linear relation between σ_o and $1/1-f^2$, which is confirmed by the numerical calculations, as shown in Fig. (5.1).

It was also confirmed that the temperature dependence of f is given by the expected linear function of $\ln T$, as shown in Fig. (5.2).

Figure 5.1 Typical Variation of f with σ_0

Figure 5.2 Representative Dependence of f_c on $\ln T$ for U-238 Capture

The capture cross section self-shielding factors for U-238 for the Bondarenko set group structure are tabulated for various values and temperatures in Table 5.2. Similar calculations were also done for the FTR-300 30-group set structure; results for the two values bracketing the composition range for LMFBR blankets are presented in Table (5.3).

Based upon these results it was concluded that the calculated self-shielding factors, and their dependence on σ_0 and temperature are in good agreement with the previously published results of other investigators. Hence we have established a good base for the case of homogeneous self-shielding upon which we can now proceed to impose the effects of heterogeneity.

5.1.3 Unit Cell Fluxes

The heterogeneous group cross section formula is derived by considering a unit cell typical of an FBR. It can be shown that the heterogeneous group macroscopic cross section Σ_{xk} for the k^{th} resonance for nuclear process x is

$$\bar{\Sigma}_{xk} = \frac{\int_{\Delta E} [V_f \Sigma_{xf}(E) \bar{\phi}_f(E) + V_c \Sigma_{xc}(E) \bar{\phi}_c(E)] dE}{\int_{\Delta E} V_{\text{cell}} \bar{\phi}_{\text{cell}}(E) dE} \quad (5.8)$$

TABLE 5.2

f_c Factors for Bondarenko Set Group Structure

in the Resolved Resonance Region

- Capture Cross Section Self-Shielding Factors for U-238 -

Group	Temp °K	σ_0	$= 10^4$	10^3	10^2	10^1	0
13	300.		0.993	0.941	0.717	0.450	0.364
	600.		0.994	0.954	0.760	0.498	0.410
	1200.		0.996	0.965	0.801	0.551	0.455
14	300.		0.988	0.907	0.627	0.367	0.292
	600.		0.991	0.927	0.675	0.410	0.329
	1200.		0.993	0.944	0.724	0.459	0.372
15	300.		0.977	0.830	0.452	0.215	0.157
	600.		0.982	0.865	0.505	0.246	0.178
	1200.		0.987	0.895	0.563	0.283	0.205
16	300.		0.961	0.746	0.346	0.154	0.115
	600.		0.971	0.793	0.394	0.177	0.123
	1200.		0.978	0.835	0.449	0.204	0.148
17	300.		0.804	0.401	0.123	0.053	0.038
	600.		0.838	0.444	0.135	0.056	0.040
	1200.		0.871	0.502	0.153	0.061	0.043
18	300.		0.811	0.381	0.124	0.061	0.069
	600.		0.848	0.429	0.139	0.065	0.072
	1200.		0.881	0.487	0.160	0.071	0.075
19	300.		0.594	0.198	0.055	0.028	0.025
	600.		0.646	0.209	0.057	0.028	0.025
	1200.		0.701	0.240	0.060	0.029	0.025
20	300.		0.702	0.219	0.061	0.027	0.021
	600.		0.780	0.250	0.065	0.028	0.021
	1200.		0.756	0.292	0.071	0.029	0.022
21	300.		0.699	0.252	0.093	0.029	0.021
	600.		0.743	0.281	0.099	0.029	0.021
	1200.		0.788	0.320	0.105	0.030	0.021

TABLE 5.3

f_c Self-Shielding Factors for FTR-300 Group Structure
 - Capture Cross Section Self-Shielding Factors for U-238 -

Group	Temp °K	σ_0	=	100.0	20.0
18	300			0.741	0.530
	600			0.785	0.581
	1200			0.826	0.636
19	300			0.798	0.608
	600			0.835	0.663
	1200			0.869	0.717
20	300			0.673	0.476
	600			0.722	0.521
	1200			0.765	0.570
21	300			0.706	0.502
	600			0.749	0.552
	1200			0.791	0.604
22	300			0.629	0.420
	600			0.676	0.467
	1200			0.724	0.519
23	300			0.511	0.314
	600			0.562	0.353
	1200			0.616	0.398
24	300			0.456	0.259
	600			0.511	0.297
	1200			0.571	0.342
25	300			0.398	0.221
	600			0.448	0.254
	1200			0.503	0.294
26	300			0.209	0.110
	600			0.235	0.123
	1200			0.267	0.139
27	300			0.111	0.054
	600			0.124	0.058
	1200			0.142	0.064
28	300			0.059	0.032
	600			0.062	0.032
	1200			0.067	0.033
29	300			0.074	0.037
	600			0.077	0.038
	1200			0.083	0.039

where

$$\bar{\phi}_\alpha(E) = \frac{1}{V_\alpha} \int_{V_\alpha} d\underline{r} \phi_\alpha(\underline{r}, E) \quad (5-9)$$

and the subscript stands for either fuel or coolant, as appropriate,

V_f , V_c , V_{cell} are the volume of fuel pin, coolant and the cell, respectively,

$\Sigma_{xf}(E)$, Σ_{xc} are the resonance cross section of the fuel pin and the non-resonant cross section of the surrounding coolant (including homogenized cladding), respectively, and

$\bar{\phi}_{\text{cell}}$ is the unperturbed cell flux.

In order to evaluate Eq. (5-8), a new function, R , is defined such that

$$R \equiv R(Q, \tau_f(E), \tau_c(E)) = \frac{\bar{\phi}_c(E)}{\bar{\phi}_f(E)} \quad (5-10)$$

where

Q is the fraction of the total neutron source introduced (by elastic moderation) in one of the two media comprising the unit cell

$\tau(E)$ is the optical thickness of the coolant (c) or fuel (f).

The volume-averaged fuel flux is calculated in a manner similar to that for the homogeneous case, and one finds that:

$$\phi_f(E) = \frac{C_o(E_o/E)^n}{V \Sigma_f R_k + V \Sigma_c R} \quad (5-11)$$

where all parameters are defined in the preceeding section.

Equation (5-11) is then inserted in Eq. (5-8) to give:

$$\bar{\Sigma}_{xk} = \frac{\int \frac{\Sigma_{xf}(E)}{\Sigma_{Rf}(E) + \frac{V_c}{V_f} \Sigma_{xc} R} \frac{dE}{E^n}}{\frac{1}{\Sigma_o} \int \frac{dE}{E^n}} \quad (5-12)$$

where

Σ_o is the total non-resonant macroscopic removal cross section (including potential scattering by the resonance absorber)

In order to calculate the flux ratio, R , typical unit cells were considered and integral transport theory used to show that for a narrow group in energy space, in which all interactions cause removal of neutrons born according to a uniform spatial distribution in each region:

$$R = \frac{\bar{\phi}_c}{\bar{\phi}_f} = \frac{1 + \left(\frac{K_{cc}}{K_{cf}} - 1\right) Q_c}{1 + \left(\frac{K_{ff}}{K_{cf}} - 1\right) Q_f} \quad (5-13)$$

where

K_{cc} , K_{ff} , K_{cf} are region-averaged transport kernels, and
 Q_c , Q_f are the fractions of the total source in the
 coolant and fuel regions, respectively.

The source fractions, Q_c and Q_f , are calculated in terms
 of the optical thickness, using continuous slowing down theory and
 the assumption of spatially uniform flux far above the resonance:

$$Q_c = \frac{\xi_c \tau_c}{\xi_c \tau_c + \xi_f \tau_{of}} \quad (5-14)$$

where

ξ_c and ξ_f are the lethargy gain per collision for coolant
 and fuel material respectively; it was found
 that only elastic scattering need be considered
 in the range of interest.

A transmission probability method for calculating the flux
 ratio, R , was also discussed, and a relation similar in form to

Eq. (5-13) was derived. Since the escape probabilities can be easily calculated at small or large optical thicknesses, it is possible to derive limiting case results for the expression. For the cells of interest the coolant region is optically thin; thus, based on these findings, the following expression was adopted for the flux ratio:

$$R = \frac{1 + \omega \tau_{af} Q_c}{1 + (1/3) \tau_{cf} Q_f} \quad (5-15)$$

where

τ_{af}, τ_c are the optical thicknesses of the fuel pin and

the coolant respectively ($\tau = \Sigma \cdot \bar{\ell}$; $\bar{\ell} = 4V/S$,

the Dirac chord length)

ω is the slope of R with respect to the optical

thickness of the fuel pin; and

$$1/3 \leq \omega \leq 2/3$$

In the present work it was shown that the $\omega = 1/3$ limit could be used for both fuel and coolant - an important simplification.

In order to verify the functional form and quantitative validity of Eq. 5-15 a numerical study of flux ratios in unit cells (both square and hexagonal) was carried out using Monte Carlo methods as well as S_8 transport methods (cylindrical cells only). As can be seen in Fig. (5.3) the flux ratio is a linear function of the source

Figure 5.3 Effect of Source Fraction on Flux Ratio

fraction as predicted by Eq. (5-15); and the upper (2/3) and lower (1/3) bounds for the slope, ω , are also confirmed, as illustrated in Fig. (5.4). It was also shown that the flux ratio is insensitive to fuel or coolant scattering without removal for scattering optical thickness $\tau_s \lesssim 2.0$, and that optical thickness is the only variable needed to characterize cell geometry.

It is interesting to note that the S_0 transport methods gave results similar in shape (functional dependence) but different in absolute values - a result attributed to the well-known inherent error in cylindricalization.

5.1.4 Heterogeneous Self-Shielding

After determining and validating the required expression for the flux ratio, the heterogeneous group cross sections could be calculated. Using Eq. (5-12), and for the capture process:

$$\bar{\sigma}_{\text{het}} = \frac{\sigma_r}{\Delta u} \frac{\Gamma_Y}{2E_r} \int_{-\infty}^{\infty} \frac{\Psi(x,t)}{\Psi(x,t) + \Phi\chi(x,t) + \bar{\beta} + \beta R(x,Q)} dx \quad (5-16)$$

where

$\bar{\beta}$ is the ratio of the non-resonant removal cross section of the fuel pin per absorber nucleus to the maximum removal cross section at the resonance peak of the resonant absorber

β is the ratio of the non-resonant removal cross section of

Figure 5.4 Flux Ratio versus Optical Thickness

the coolant per absorber nucleus to the maximum removal cross section at the resonance peak of the resonant absorber, and

other parameters are defined in the preceeding sections.

Note that Eq. 5-16 reduces to the homogeneous case, Eq. 5-4, when $R \equiv 1.0$: heterogeneity merely acts to increase the relative importance of neutrons removed by the coolant.

Equation (5-10) is inserted into Eq. (5-15) and then divided by the infinite dilution cross section to obtain the self-shielding f factor:

$$f_{\text{het}}(B) = \frac{B/B'}{\pi(1 + \delta)} \cdot \int_{-\infty}^{\infty} \frac{B'\Psi(x,t)}{\Psi(x,t) + \Phi\chi(x,t) + B'} dx \quad (5-17)$$

where

$$B = \beta + \bar{\beta} \quad (5-18)$$

$$B' = \bar{\beta} + \frac{\beta}{(1 + (1/3)\tau_c Q_f) \cdot (1 + \frac{\beta \omega \bar{\ell}_f \Sigma_r Q_c}{1 + (1/3)\tau_c Q_f})} \quad (5-19)$$

$\bar{\ell}_f$ is the mean (Dirac) chord length through the fuel pin and ω is assumed constant.

The relation between the homogeneous and heterogeneous self-

shielding factors is then given by the new equivalence relation:

$$\frac{f_{\text{het}}(B)}{f_{\text{hom}}(B)} = \frac{B/B'}{1 + \delta} \frac{f_{\text{hom}}(B')}{f_{\text{hom}}(B)} \quad (5-20)$$

or, in terms of the coolant optical thickness and source fractions

$$\frac{f_{\text{het}}(\sigma_o)}{f_{\text{hom}}(\sigma_o)} = \frac{\frac{\sigma_o + \sigma_{pa}}{\sigma_o' + \sigma_{pa}}}{1 + \frac{\omega \tau_c Q_c}{1 + (1/3)\tau_c Q_f}} \cdot \frac{f_{\text{hom}}(\sigma_o')}{f_{\text{hom}}(\sigma_o)} \quad (5-21)$$

where

σ_o' is the value of σ_o modified to account for heterogeneity and

$$\sigma_o' = \sigma_o - \frac{(1/3)\tau_c^2}{1 + (1/3)\tau_c} \cdot \frac{1}{(\bar{\ell}_f N_o)} \quad (5-22)$$

where N_o is the absorber concentration, nuclei/barn cm, in the fuel region.

Although this relation was developed for a single resonance it can be applied to a broad group in a multigroup set because none of the parameters involved vary appreciably over the energy range involved. Similarly, the derivation has focused on the capture reaction in U-238, but also applies to self-shielding of scattering interactions and to other nuclei.

5.1.4.1 Approximate Forms for the Equivalence Relations

Equation (5-20) can be developed into a simpler, but still quite useful prescription. The results are particularly useful in that they clarify a basic ambiguity in the narrow resonance approximation.

We have

$$\frac{B/B'}{1+\delta} = \frac{1}{1 + \delta(1 - \frac{Q_c^*}{Q_c})} \quad (5-23)$$

and by expanding the self-shielding factor $f_{\text{hom}}(B')$ into a Taylor series around B and using Eq. (5-7) for the relation between f and σ_o , one gets

$$\frac{f_{\text{hom}}(B')}{f_{\text{hom}}(B)} = 1 - (1/2)(1 - f_{\text{hom}}^2(B)) \frac{\delta}{1 + \delta} \frac{Q_c^*}{Q_c} \quad (5-24)$$

where

$$Q_c^* = \beta/B = \frac{\sigma_{oc}}{\sigma_o + \sigma_{pa}} \quad (5-25)$$

and

σ_{oc} is the coolant contribution to σ_o .

The final form can be expressed in terms of the optical thickness of the coolant and the source fraction,

$$\frac{f_{het}(\sigma_o)}{f_{hom}(\sigma_o)} = 1 - (1/3)\tau_c Q_c \left[1 - \frac{1 + f_{hom}^2(\sigma_c) \frac{Q_c^*}{Q_c}}{2} \right]$$

(5-26)

However, the form given by Eq. (5-26) does not correctly reproduce obvious limiting cases (e.g. f_{hom} should approach f_{hom} when f_{hom} approaches 1.0).

Because of this failure, the flux ratio expression was re-examined and it was shown that the most logical way to obtain a flat spatial flux ($R = 1$) far from the peak of a resonance, is to allow only the resonance part of the total cross sections to remove neutrons (the non-resonant or background cross sections can be regarded as scattering as many neutrons into a given dE about E as they scatter out). Thus τ_{af} in Eq. (5-16) was replaced by $(\tau_{af} - \tau_{0_f})$ where τ_{0_f} is the non-resonant contribution; Eq. (5-15) becomes (using $\omega = 1/3$; see discussion subsequent to Eq. 5-30):

$$R = 1 + 1/3 (\tau_{af} - \tau_{0_f}) Q_c \quad (5-27)$$

Following exactly the same steps as before, the equivalence theorem corresponding to Eq. (5-17) becomes

$$f_{het}^{(B)} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\tilde{B}\Psi(x,t)}{\Psi(x,t) + \Phi_X(x,t) + \tilde{B}} dx \quad (5-28)$$

where

$$\tilde{B} = \frac{B}{1 + (1/3)\tau_c Q_c} \quad (5-29)$$

and the simplified version corresponding to Eq. (5-26) becomes

$$\frac{f_{het}(\sigma_o)}{f_{hom}(\sigma_o)} = 1 - (1/6)(1 - f_{hom}^2(\sigma_o))\tau_c Q_c \quad (5-30)$$

In the above calculations the slope, ω , was taken to be 1/3. When the difference between the integrands of the homogeneous and heterogeneous f factors, ΔI , is plotted versus the reduced energy, x , as seen in Fig. (5-5), the case with $\omega = 1/3$ is in much better agreement with the "exact" case.

It is interesting to note that the equivalence relation we have obtained here is possible only if a linear functional relation of the form of Eq. (5-15) with constant ω is employed.

5.1.4.2 Numerical Verification and Applications

The heterogeneous effects in two types of FBR unit cells were examined by applying the expressions just derived to three representative resonances contained in the narrow energy groups whose properties are given in Table 5.4.

The effects of heterogeneity on the self-shielding f factors

Figure 5.5 The Effect of Flux Ratio Slope on the Heterogeneous Integrand

TABLE 5.4

The Energy Group Structure of the Three
Representative Energy Groups

Group	Upper Energy (eV)	Lower Energy (eV)	Resonance Energy (eV)
1	1100	1000	1054
2	150	80	102.6
3	12	2	6.67

of a representative UO_2 cell (radial blanket cell representative of that used in the MIT Blanket Test Facility) were calculated using the CIDI program. The results are shown in Table 5.5. Note that a slope of $1/3$ for the flux ratio produces results in much better agreement with the "exact" case. The "exact" slope, $\omega(\tau_{af})$, is the slope fitted to the Monte Carlo results presented in the previous section. A similar computation was applied to a metal-fueled blanket cell (representing the cell structure of the standard MIT-BTF radial blanket assemblies); the results are presented in Table 5.6. As seen in Tables 5.5 and 5.6 the heterogeneous effects are smaller than typical uncertainties in the cross sections.

In order to determine the effects of heterogeneity on some important integral properties of a FBR, multigroup calculations were carried out in which the shielding level (σ_0) was changed from an unshielded case ($\sigma_0 = \infty$) to a totally shielded case ($\sigma_0 = 0$). The results shown in Table 5.7 demonstrated that the effect on the breeding ratio is negligible for typical FBR's, where heterogeneity would change σ_0 by less than 1 barn from its homogeneous value of approximately 25 barns.

Heterogeneous effects in the core and in GCFR assemblies are even smaller than those considered above, since radial blankets in an LMFBR have a higher Q_c and τ_c than in a GCFR, and also employ larger diameter rods than the core.

TABLE 5.5

Effects of Heterogeneity on U-238 Capture Self-Shielding Factor
 for Three Energy Groups for a UO_2 Fueled Unit Cell
 (All Data Calculated Using CIDI Program)

$$\text{Ratio} = \frac{f_{\text{het}}}{f_{\text{hom}}}$$

Group	Homogeneous f_c	ω			Approximate Values	
		1/3	"exact"	2/3	Eq (5-25)	Eq (5-29)
1	0.198	0.989	0.986	0.974	0.9906	0.9902
2	0.0437	0.992	0.987	0.979	0.9902	0.9898
3	0.0386	0.992	0.987	0.978	0.9902	0.9898

TABLE 5.6

Effects of Heterogeneity on U-238 Capture Self-Shielding Factor
 for Three Energy Groups for a Metal-U-Fueled Unit Cell
 (All Data Calculated Using CIDI Program)

$$\text{Ratio} = \frac{f_{\text{het}}}{f_{\text{hom}}}$$

Group	Homogeneous f_c	ω			Approximate Values	
		1/3	"exact"	2/3	Eq (5-25)	Eq (5-29)
1	0.19 8	0.976	0.973	0.953	0.9796	0.9833
2	0.0437	0.977	0.972	0.959	0.9791	0.9827
3	0.0386	0.979	0.972	0.958	0.9791	0.9827

TABLE 5.7

Radial Blanket Breeding Ratio as a Function of U-238 Self-Shielding
in the Blanket for Two Different Degrees of Shielding in the Core

σ_0 in the Blanket	Radial Blanket Breeding Ratio			
	for Core	System	for Core	System
	$\sigma_0 = 0$	k	$\sigma_0 = 100$	k
∞	0.26	1.138	0.28	1.085
10^4	0.26	1.138	0.28	1.085
10^3	0.26	1.139	0.28	1.086
10^2	0.25	1.141	0.28	1.086
10^1	0.23	1.144	0.25	1.101
0	0.22	1.146	0.24	1.103

5.2 Conclusions

Based upon the work reported here the following conclusions are substantiated:

- (1) A new and easily applied equivalence theorem, summarized in Table 5.8, has been developed for fast reactor applications, and can be applied to any available sets of homogeneous self-shielding factors tabulated as a function of σ_0 , the background cross section per resonance absorber (or scatterer) nucleus.
- (2) A simple prescription, adequate for most purposes (again see Table 5.9) has been developed from the more general result.
- (3) In any event, the corrections for heterogeneity appear to be negligible for fast reactors: on the order of several percent at the most, much smaller than typical uncertainties in basic cross section data.
- (4) In particular, heterogeneity corrections do not have any important effect on the calculated breeding performance of blanket mock-ups studied in the MIT Blanket Test Facility, even though there is a difference between the heterogeneous corrections for the metal and oxide-fueled subassemblies employed.

TABLE 5.8

SUMMARY OF EQUIVALENCE THEOREM FOR RESONANCE SELF-SHIELDING IN FBR's*

1. The ratio of the heterogeneous to homogeneous self-shielding factor (using the Bondarenko formulations) for a given group in a multi-group cross section set is given by (renormalized version - note difference from Eq. 5-21, the un-normalized version)

$$\frac{f_{\text{het}}(\sigma_o)}{f_{\text{hom}}(\sigma_o)} = \frac{f_{\text{hom}}(\sigma_o')}{f_{\text{hom}}(\sigma_o)} \quad (5-31)$$

where

σ_o is the background nonresonant cross section for the homogeneous cell, barns per resonant absorber (scatterer) nucleus

σ_o' is the background non resonant cross sections for the heterogeneous cell and

$$\sigma_o' = \left[\frac{1 - (1/3)\tau_c Q_c \frac{\sigma_{pa}}{\sigma_o}}{1 + (1/3)\tau_c Q_c} \right] \cdot \sigma_o \quad (5-32)$$

2. A simple version derived from the above is:

$$\frac{f_{\text{het}}(\sigma_o)}{f_{\text{hom}}(\sigma_o)} = 1 - (1/6)(1 - f_{\text{hom}}^2(\sigma_o))\tau_c Q_c \quad (5-33)$$

*See Appendix B for a numerical example

TABLE 5.8 (continued)

where

$$\tau_c = N_c \sigma_{R_c} \bar{l}_c \quad (5-34)$$

$$Q_c = \frac{\xi_c \tau_c}{\xi_c \tau_c + \xi_f \tau_{0f}} \quad (5-35)$$

and $\bar{l}_c$ is the mean Dirac chord length of the coolant region, $4V/S$.

5.3 Recommendations for Future Work

As a consequence of the results obtained in this research, the following work should be considered for the future:

- (1) The utility of the simple coolant-to-fuel flux ratio prescription in other applications should be investigated; for example:

- (a) for calculation of first flight effects involving fast neutron removal
- (b) as a module in codes to calculate thermal neutron spectra

For this purpose the prescription should be improved by:

- (c) developing a convenient curve-fit between the $\omega = 1/3$ and $2/3$ asymptotes
 - (d) including quantitative corrections for scattering without removal
 - (e) developing similar expressions for the flux at the cell periphery and the coolant/clad interface
- (2) The results obtained here for resonance absorption should be extended to
 - (a) other geometries - particularly the slab geometry used in fast critical assemblies
 - (b) other reactor types - thermal reactors in particular
 - (c) other resonance treatments: wide and intermediate resonances, and unresolved resonances.

- (3) Thompson (T3) has measured and Gregory (G6) has discussed the relation between experimentally measured U-238 capture rate profiles through fuel rods and self-shielding factors. This subject should be reinvestigated in the light of the present results to demonstrate the compatibility between theory and experiment.

All of the above activities appear to be feasible extensions of what has been accomplished to date, given sufficient attention. However, the effects of the abrupt variation in self-shielding near the blanket-reflector interface, which have been observed in blanket foil activation traverses at MIT, also need to be investigated, and analytic means found to incorporate this effect in multigroup calculations. Unfortunately the present work has given no clear indication of how to proceed on this latter task.

APPENDIX A

The CIDI Computer Code

In this appendix, a listing of the CIDI computer code is given, together with some interpretive remarks and a sample input and output. This was thought to be worthwhile because of the central role of CIDI in the work reported here, and because of shortcomings encountered in published versions of similar programs which might be used for the same purpose. It should be noted, however, that CIDI was designed to be a research tool and not a production program.

CIDI calculates the group-averaged cross sections in the resolved resonance range for a specified isotope. The code can be used for both homogeneous and heterogeneous systems. The code requires as input the dimensions of an equivalent cylindrical cell, the non-resonant cross sections of the unit cell material, the resonance parameters of the resonance absorber, and the energy group structure. The code uses Eq (3-12) along with Eqs (2-26), (2-27), and (2-28) to calculate the group cross sections. The Voigt shape

functions in these equations are calculated with subroutine PSIXI, which is taken from the MIGROS-2 code (H5) (note, however, that it was found necessary to correct PSIXI, hence the version listed here differs from that in MIGROS-2). The energy integral is evaluated numerically by the QAR subroutine from IBM's copyrighted SLMATH.SUBR package (I2).

A.1 Subroutine PSIXI

Due to a major error in this subroutine, an explicatory note is called for. Subroutine PSIXI is taken from the computer code MIGROS-2 (H5). This subroutine uses the method derived by Chiarella and Reichel (C2). In this method, the Fourier transforms of $\psi(x,t)$ and $\chi(x,t)$ are taken to form a complex function. Then, with the aid of the theorems of complex analysis, series approximations to the above-mentioned functions are developed. (Note a (hopefully obvious) typographical error in Eq (2.2) of (C2), a missing factor of 2 .)

The subroutine PSIXI uses these series representations of the $\psi(x,t)$ and $\chi(x,t)$ functions. Unfortunately, the series is prematurely truncated when the original form of the subroutine is used. By merely removing one card from the subroutine and thus allowing other terms of the series to enter into the calculation, this error was corrected, and the resulting $\psi(x,t)$ function was found to be in excellent agreement with tabulated values of

$\psi(x,t)$ (S4). Thus it is recommended that our version of PSIXI
(see listing) be adopted for future efforts.

A.2 Input to CIDI

Variable		Description
ENTRY1	TITLE(18) 18A4 Format	Identification
ENTRY2	Namelist NACIS	
	NBG	Number of broad groups
	NB1	Number of the first broad group
	NBL	Number of the last broad group
	IREP	0 single run 1 multiple run for different cell parameters
	IREPA	0 single run 1 multiple runs for different resonance parameters
	IWRITE	0 does not print inter- mediate steps 1 print intermediate steps
	IPUNCH	0 no punch output 1 group cross-sections are punched out

(The following order repeats NBG times.)

ENTRY3	Namelist ECE	
	IBG	Number of the broad group
	XEU	Upper energy of the group
	XEL	Lower energy of the group
	INR	Number of resonances in the group

PDEN	Number density of the non-resonant elements in the fuel region (nuclei/barn-cm)
RDEN	Number density of the resonant absorber in the fuel region (nuclei/barn-cm)
RF	Radius of the fuel pin, in cm
RC	Outer radius of the cylindricized cell, in cm
A	Atomic number of the resonance absorber
AM	Atomic number of the coolant material
AMI	Atomic number of the non-resonant element in the fuel region
IQ	0 All sources are in the coolant 1 Source ratio is calculated
IRATIO	1 Homogeneous calculation 2 Heterogeneous calculation
TEMP	Temperature of the medium in ° K
IN	Initial width of the fine group in terms of total resonance width, usually 10
LMN	A parameter of the inte- gration subroutine, usually 10

A.3 Output from CIDI

The format of the output depends on the IWRITE and IPUNCH variables in namelist NACIS. If IWRITE = 0 , then the code writes the essential information and the final cross-sections of all the groups. If IPUNCH = 1 then the final cross sections are punched.

Following is a description of the output of CIDI.

- IPUNCH = 1 Code punches out the temperature and σ_0 used in the calculation along with the cross-section of NRG groups, according to (E12.5/E12.5) (3E2.5,10X,I3) format.
- IWRITE = 0 On the first page, general information from namelists NACIS and MINE is printed. Then for every group, the number density ratios, σ_0 for the group, volume ratio, coolant optical thickness, average lethargy gain per collision for fuel and coolant regions along with the cross-sections of the two regions are printed. The summary of all the group cross sections are then printed with and without corrections due to the resonance tails.
- IWRITE = 1 Under this option, in addition to the above output, for every group the ECE namelist and the resonance parameters are printed along with the source ratio for the group. Then for each resonance various parameters in

Eq (2-5) to Eq (2-11) are printed.

A.4 Listing of CIDI (follows on succeeding pages)

THIS PROGRAM CALCULATES SELF-SHIELDED RESONANCES CROSS SECTIONS FOR A
CYLINDRICAL UNIT CELL. NARROW RESONANCE APPROXIMATION AND SINGLE LEVEL
BREIT-WIGNER RESONANCE FORMULA ARE USED.

THE INPUT TO THE CODE IS MADE OF THREE PARTS.

- 1- ENERGY GROUP STRUCTURE
- 2- RESONANCE PARAMETERS
- 3- NON-RESONANT CROSS SECTIONS AND THE DIMENSION OF THE CELL

THE MAIN PROGRAM CONTROLS THE FLOW OF THE CALCULATIONS. PREPARES THE
VARIOUS PARAMETERS AND CALLS SUBROUTINES.

```

REAL MDEN
INTEGER BG,BG1,BGL,BGG
COMMON/CE/RF,RC,MDEN,PCEN,RDEN,TAUC,TEMP,A
COMMON/CR/E(150),GN(150),GG(150),G(150),EK(150),EM(150),BG,EU,EL,
1NR,XN,IN
COMMON/CC/SIGAM,SIGSM,SGBSMF,SGBAMF,SGAF,SGSF,V,W,WC,RO,XIF,XIM
COMMON/CWR/ IWRITE
COMMON/CER/ IBG(13),XEU(13),XEL(13),XNX(13),INR(13),XYZ(4,13,150),
1BGG,ZYX(3,13,150)
COMMON/CLMN/ LMN,IQ
COMMON/CRAT/ IRATIO
DIMENSION TITLE(18)
DIMENSION KK(13),CROSS(13),CROSA(13),CROST(13),TESIR(13)
DIMENSION SGMA(13),SGMS(13),SGBFS(13),SGBFA(13),SGFA(13),SGFS(13)

```

THIS NAMELIST DEFINES THE ENERGY GROUP STRUCTURE.

NAMELIST/NACIS/NBG,BG1,BGL,IREP,IWRITE,IREPA,IPUNCH

MAIN0001
 MAIN0002
 MAIN0003
 MAIN0004
 MAIN0005
 MAIN0006
 MAIN0007
 MAIN0008
 MAIN0009
 MAIN0010
 MAIN0011
 MAIN0012
 MAIN0013
 MAIN0014
 MAIN0015
 MAIN0016
 MAIN0017
 MAIN0018
 MAIN0019
 MAIN0020
 MAIN0021
 MAIN0022
 MAIN0023
 MAIN0024
 MAIN0025
 MAIN0026
 MAIN0027
 MAIN0028
 MAIN0029
 MAIN0030
 MAIN0031
 MAIN0032
 MAIN0033
 MAIN0034
 MAIN0035
 MAIN0036

```

C      THIS NAMELIST DEFINES RESONANCE PARAMETERS FOR EACH RESONANCE SEPARATELY
C
C      NAMELIST/ECE/IBG,XEU,XEL,INR,XNX
C
C      THIS NAMELIST DEFINES NONRESONANT CROSS SECTIONS,AND THE PROPERTIES OF
C      THE CELL.
C
      NAMELIST/MINE/SGMA,SGMS,SGBFS,SGBFA,SGFA,SGFS,RC,RF,AM,A,MDEN,IQ,
      IPDEN,RDEN,TEMP,IN,AMI,LMN,IRATIO
      EXTERNAL EPART
1  FORMAT(2X,'COOLANT DENSITY=',E12.5/' FUEL PIN DENSITY=',E12.5/2X,
1' FUEL-PIN ABS. DENSITY=',E12.5///2X,' FUEL-PIN RADIUS=',E12.5,
25X,'UNIT CELL OUTER RADIUS=',E12.5///2X,'TEMP=',E12.5///)
2  FORMAT(2X,'NC/N28=',E12.5,' N/N28=',E12.5,' SIG-N/RDEN=',E12.5/
3 2X,
1'VOL. RATIO=',E12.5,' COOLANT OPT. THICKNESS=',E12.5/2X,'XIM=',
2E12.5,' XIF=',E12.5//)
4  FORMAT(4X,I3,2X,E12.5,2X,E12.5,2X,E12.5)
10 FORMAT(10X,'HOMOGENEOUS UNIT CELL CALCULATION'////////)
11 FORMAT(2X,'IN=',I4,' IREP=',I2,' IREPA=',I2,' IWRITE=',I2,
1' IPUNCH=',I2,' IRATIO=',I2,' IQ=',I2////////)
12 FORMAT(10X,'HETEROGENEOUS UNIT CELL CALCULATION'////////)
13 FORMAT(2X,'COOLANT ABS.X-SECTION=',E12.5,
12X,'COOLANT SCAT. X-SECTION=',E12.5/2X,
2' FUEL-PIN NON-RESON. ABS. X-SECTION=',E12.5,2X,
3' FUEL-PIN NON-RESON. SCAT X-SECTION=',E12.5/2X,
4' FUEL-PIN NON-RESON. ABS. X-SECTION FOR ABS.NUC.=',E12.5,2X,
5' FUEL-PIN NON-RESON. SCAT X-SECTION FOR ABS.NUC.=',E12.5///)
44 FORMAT(2X,'GROUP',4X,' SIGMA-ABS.',4X,' SIGMA-SCT.',4X,' SIGMA-TOT.',
1,/)
53 FORMAT(2X,'DDD=',E12.5)
54 FORMAT(///,2X,'BRAVO YOU REACH THE END OF CIDI ')
56 FORMAT(4E12.5)
57 FORMAT(E12.5/E12.5/(3E12.5,10X,I3))
58 FORMAT(2X,'NUMBER OF BROAD GROUPS=',I6,10X,'FIRST BROAD GROUP=',I3

```

```

MAIN0037
MAIN0038
MAIN0039
MAIN0040
MAIN0041
MAIN0042
MAIN0043
MAIN0044
MAIN0045
MAIN0046
MAIN0047
MAIN0048
MAIN0049
MAIN0050
MAIN0051
MAIN0052
MAIN0053
MAIN0054
MAIN0055
MAIN0056
MAIN0057
MAIN0058
MAIN0059
MAIN0060
MAIN0061
MAIN0062
MAIN0063
MAIN0064
MAIN0065
MAIN0066
MAIN0067
MAIN0068
MAIN0069
MAIN0070
MAIN0071
MAIN0072

```

```

1, ' LAST BROAD GROUP=', I3//2X, 'SOURCE RATIO IN THE FUEL RCD=', I2,
8, '(IQ=1 SOURCE RATIO IS CALCULATED, IQ=0 ALL SOURCES ARE IN THE ',
9, 'COOLANT)'//2X, 'FLUX RATIO=', I2,
2, '(IRATIO=1, HOMOGENEOUS, OTHERS HETEROGENEOUS)'//2X,
3, 'INTEGRATION HALF WIDTH=', I5, '*GAMMA', I0X, 'EXPONENT OF 2 FOR THE '
4, 'INTEGRATION SUBROUTINE=', I2//2X, 'IREP=', I2, 5X, 'IREPA=', I2//2X,
5, 'IWRITE=', I2, '(IF 1 PRINTS RESULTS BY RESONANCE, IF NOT PRINTS ',
6, 'ONLY THE FINAL RESULTS)'//2X, 'IPUNCH=', I2, '(IF 1 PUNCHES THE ',
7, 'FINAL RESULTS)'///)
9999 FORMAT(1H1)
1233 FORMAT(20X, 18A4///)
1234 FORMAT(18A4)
      READ(5, 1234) TITLE
      WRITE(6, 1233) TITLE
      IREP=0
      IREPA=0
      IRATIO=1
      IWRITE=1
      IPLNCH=1
      IQ=2
      PI=3.14156
88 READ(5, NACIS)
      BGG=BGL-BG1+1
      DO 55 KKK=1, BGG
      READ(5, ECE)
      NR=INR(KKK)
      READ(5, 56) ((XYZ(J, KKK, L), J=1, 4), L=1, NR)
55 CONTINUE
99 WRITE(6, 9999)
      READ(5, MINE)
      IF(IRATIO.EQ.1) WRITE(6, 10)
      IF(IRATIO.NE.1) WRITE(6, 12)
      WRITE(6, 1) MDEN, PDEN, RCEN, RF, RC, TEMP
      WRITE(6, 58) NBG, BG1, BGL, IQ, IRATIO, IN, LMN, IREP, IREPA, IWRITE, IPUNCH
C
C HERE THE NECESSARY PARAMETERS OF THE CELL ARE CALCULATED.

```

```

MAIN0073
MAIN0074
MAIN0075
MAIN0076
MAIN0077
MAIN0078
MAIN0079
MAIN0080
MAIN0081
MAIN0082
MAIN0083
MAIN0084
MAIN0085
MAIN0086
MAIN0087
MAIN0088
MAIN0089
MAIN0090
MAIN0091
MAIN0092
MAIN0093
MAIN0094
MAIN0095
MAIN0096
MAIN0097
MAIN0098
MAIN0099
MAIN0100
MAIN0101
MAIN0102
MAIN0103
MAIN0104
MAIN0105
MAIN0106
MAIN0107
MAIN0108

```

C

$W = MDEN / RDEN$
 $WC = PDEN / RDEN$
 $V = (RC / RF) * (RC / RF) - 1.$
 $VF = PI * RF * RF$
 $VC = PI * (RC * RC - RF * RF)$
 $VCEL = VC + VF$
 $ZRF = (RC * RC - RF * RF) / RF$
 $XIM = 2. / (AM + 2. / 3.)$
 $KK(1) = BGI$

C
C
C
C

STARTING THE CROSS SECTION CALCULATION.
 BROAD GROUPS ARE CONSIDERED .

$DO\ 3\ K=1, BGG$
 $BG = IBG(K)$
 $NR = INR(K)$
 $EU = XEU(K)$
 $EL = XEL(K)$
 $XN = XNX(K)$
 $SIGAM = SGMA(K)$
 $SIGSM = SGMS(K)$
 $SGBSMF = SGBFS(K)$
 $SGBAMF = SGBFA(K)$
 $SGAF = SGFA(K)$
 $SGSF = SGFS(K)$
 $XIF1 = 2. / (AM1 + 2. / 3.)$
 $XIF = 2. / (A + 2. / 3.)$
 $XIF = (XIF * RDEN * SGSF + XIF1 * PDEN * SGBSMF) / (PDEN * SGBSMF + RDEN * SGSF)$
 $SIGRM = SIGAM + SIGSM$
 $SGBRMF = SGBAMF + SGBSMF$
 $SGRF = SGAF + SGSF$
 $Z = (PDEN * SGBRMF + MDEN * SIGRM * V) / RDEN$
 $TAUC = 2. * MDEN * ZRF * (SIGAM + SIGSM) * (VC / VCEL)$
 $WRITE(6, 9999)$
 $WRITE(6, 2) W, WC, Z, V, TAUC, XIM, XIF$

MAIN0109
 MAIN0110
 MAIN0111
 MAIN0112
 MAIN0113
 MAIN0114
 MAIN0115
 MAIN0116
 MAIN0117
 MAIN0118
 MAIN0119
 MAIN0120
 MAIN0121
 MAIN0122
 MAIN0123
 MAIN0124
 MAIN0125
 MAIN0126
 MAIN0127
 MAIN0128
 MAIN0129
 MAIN0130
 MAIN0131
 MAIN0132
 MAIN0133
 MAIN0134
 MAIN0135
 MAIN0136
 MAIN0137
 MAIN0138
 MAIN0139
 MAIN0140
 MAIN0141
 MAIN0142
 MAIN0143
 MAIN0144

	WRITE(6,13) SIGAM,SIGSM,SGBAMF,SGBSMF,SGAF,SGSF	MAIN0145
C		MAIN0146
C	FINE GROUPS IN A BROAD GROUP ARE CONSIDERED.	MAIN0147
C		MAIN0148
	DO 33 LM=1,NR	MAIN0149
	E(LM)=XYZ(1,K,LM)	MAIN0150
	GN(LM)=XYZ(2,K,LM)	MAIN0151
	GG(LM)=XYZ(3,K,LM)	MAIN0152
33	G(LM)=XYZ(4,K,LM)	MAIN0153
	DDC=EPART(EU,EL,XN)/(SGSF+WC*SGBSMF+W*V*SIGSM)	MAIN0154
	CALL EYCH(RATT,RATT1,K,DDD)	MAIN0155
	IF(IWRITE.GT.0) WRITE(6,53) DDD	MAIN0156
	IF(K.GE.BGG) GO TO 618	MAIN0157
619	KK(K+1)=KK(K)+1	MAIN0158
618	CROSA(K)=RATT	MAIN0159
	CROSS(K)=RATT1+SGSF	MAIN0160
	CROST(K)=CROSS(K)+CROSA(K)	MAIN0161
3	CONTINUE	MAIN0162
	WRITE(6,9999)	MAIN0163
	WRITE(6,44)	MAIN0164
C		MAIN0165
C	GROUP CROSS SECTIONS WITHOUT CORRECTIONS.	MAIN0166
C		MAIN0167
	WRITE(6,4) (KK(K),CROSA(K),CROSS(K),CROST(K),K=1,BGG)	MAIN0168
	CALL DUZELT(TESIR)	MAIN0169
	TESIR(K)=0.0	MAIN0170
	DO 5 K=1,BGG	MAIN0171
	CROSA(K)=CROSA(K)+TESIR(K)	MAIN0172
5	CROST(K)=CROST(K)+TESIR(K)	MAIN0173
	WRITE(6,44)	MAIN0174
	WRITE(6,4) (KK(K),CROSA(K),CROSS(K),CROST(K),K=1,BGG)	MAIN0175
C		MAIN0176
C	CROSS SECTIONS WITH TAIL EFFECTS INCLUDED.	MAIN0177
C		MAIN0178
	IF(IPUNCH.EQ.1)	MAIN0179
	1WRITE(7,57) TEMP,2,(CROSA(K),CROSS(K),CROST(K),KK(K),K=1,BGG)	MAIN0180

WRITE(6,9999)
IF(IREP.EQ.1) GO TO 99
87 IF(IREPA.EQ.1) GO TO 88
100 WRITE(6,54)
STOP
END

MAIN0181
MAIN0182
MAIN0183
MAIN0184
MAIN0185
MAIN0186

SUBROUTINE EYCH(RATT,RATT1,K,DDD)

THIS SUBROUTINE IS THE MOST IMPORTANT SUBROUTINE OF THE CODE, IT
CALCULATES THE RESONANCE CROSS SECTION FOR THE RESOLVED RESONANCE
REGION.

REAL MDEN
INTEGER BG
COMMON/CE/RF,RC,MDEN,PDEN,RDEN,TAUC,TEMP,A
COMMON/CR/E(150),GN(150),GG(150),G(150),EK(150),EM(150),BG,EU,EL,
INR,XN,IN
COMMON/CC/SIGAM,SIGSM,SGBSMF,SGBAMF,SGAF,SGSF,V,W,WC,RO,XIF,XIM
COMMON/CWR/ IWRITE
COMMON/CFCT/ T,SGO,SGOA,SGOS,OMEX,OMEBX,PHUX,BETA,BETAB,QQ,PHU
1,PHUXX,POT
COMMON/CGAM/GAM(150),IIN
COMMON/CER/ IBG(13),XEU(13),XEL(13),XNX(13),INR(13),XYZ(4,13,150),
1BGG,ZYX(3,13,150)
COMMON/CLMN/ LMN,IQ
COMMON/CRAT/ IRATIO
DIMENSION RR(150),GGG(150)
EXTERNAL FCT
1 FORMAT(4E12.5)
3 FORMAT(2X,'OMEX=',E12.5,' ',OMEBX=',E12.5,' ',BETA=',E12.5,
1', BETAB=',E12.5,' ',PHUX=',E12.5,' ',PHUXX=',E12.5/2X,'POT=',E12.5)
4 FORMAT(3X,'ENERGY',6X,'GAMMA-N',5X,'GAMMA-G',8X,'G'/)
6 FORMAT(2X,'BROAD GROUP=',I3,' ',# RES.=' ',I4,' ',XN=',E12.5/
12X,'UPPER ENERGY OF THE GROUP=',E12.5,
2', LOWER ENERGY OF THE GROUP=',E12.5/)
17 FORMAT(2X,' RR(',I3,')=',E12.5,30X,' IER=',I2)
18 FORMAT(2X,' GGG(',I3,')=',E12.5,30X,' IER=',I2/)
19 FORMAT(2X,'YINTA=',E12.5,2X,'YINTS=',E12.5,10X,
1'% DIFF. FROM ANALYTICAL CROSS SECTION=',E12.5)
25 FORMAT(2X,'CORREC=',E12.5,5X,'CORR=',E12.5)

EYCH0001
EYCH0002
EYCH0003
EYCH0004
EYCH0005
EYCH0006
EYCH0007
EYCH0008
EYCH0009
EYCH0010
EYCH0011
EYCH0012
EYCH0013
EYCH0014
EYCH0015
EYCH0016
EYCH0017
EYCH0018
EYCH0019
EYCH0020
EYCH0021
EYCH0022
EYCH0023
EYCH0024
EYCH0025
EYCH0026
EYCH0027
EYCH0028
EYCH0029
EYCH0030
EYCH0031
EYCH0032
EYCH0033
EYCH0034
EYCH0035
EYCH0036

```

26 FORMAT(2X,'CORREC=',E12.5)
126 FORMAT(2X,'EK(',I3,')=',E12.5,', EM(',I3,')=',E12.5,10X,'IN=',I4)
777 FORMAT(2X,'T=',E12.5,', DELTA=',E12.5,', SGO=',E12.5,', SGOA=',
1E12.5,', SGOs=',E12.5)
9999 FORMAT(///)
      IF(IWRITE.GT.0) WRITE(6,6) BG,NR,XN,EU,EL
C
C   FINE GROUP WIDTH IS DETERMINED.
C
      XIN=FLOAT(IN)
      DO 22 L=1,NR
      EK(L)=E(L)-XIN*(GN(L)+GG(L))/2.
22  EM(L)=E(L)+XIN*(GN(L)+GG(L))/2.
      IF(IWRITE.GT.0) WRITE(6,4)
      IF(IWRITE.GT.0) WRITE(6,1) (E(M),GN(M),GG(M),G(M),M=1,NR)
      IF(IWRITE.GT.0) WRITE(6,9999)
      EPS=1.0E-15
      NDIM=500
      PI=3.141596
      SIGRM=SIGAM+SIGSM
      SGBRMF=SGBAMF+SGBSMF
      VF=PI*RF*RF
      VC=PI*(RC*RC-RF*RF)
      VCEL=VC+VF
      SGRF=SGAF+SGSF+SGBSMF+SGBAMF
      XIMF=XIM/XIF
C
C   CALCULATES THE SOURCE FRACTION IN THE FUEL PIN.
C
      IF(IQ.EQ.1) GO TO 14
13  N=0
      QQ=0.0
      RO=1.00
      GO TO 53
14  QQ=1.0
      N=G

```

```

EYCH0037
EYCH0038
EYCH0039
EYCH0040
EYCH0041
EYCH0042
EYCH0043
EYCH0044
EYCH0045
EYCH0046
EYCH0047
EYCH0048
EYCH0049
EYCH0050
EYCH0051
EYCH0052
EYCH0053
EYCH0054
EYCH0055
EYCH0056
EYCH0057
EYCH0058
EYCH0059
EYCH0060
EYCH0061
EYCH0062
EYCH0063
EYCH0064
EYCH0065
EYCH0066
EYCH0067
EYCH0068
EYCH0069
EYCH0070
EYCH0071
EYCH0072

```

```

    TAUF=2.*RF*(RDEN*SGSF+PDEN*SGBSMF*(VF/VCEL))
54  RO=(1.+(1./3.)*TAUF*(1.-QQ))/(1.+(1./3.)*TAUC*QQ)
    BB8BB=XIMF*V*W*SIGSM*RO/(WC*SGBSMF+SGSF)
    QQ1=1./(1.+BB8BB)
    QQ2=QQ-QQ1
    QQ2=ABS(QQ2)-0.001
    QQ=QQ1
    N=N+1
    IF(QQ2) 53,53,54
53  IF(IWRITE.GT.0) WRITE(4,20) N,RO,QQ
20  FORMAT(2X,'N=',I6,', RC=',E12.5,', QQ=',E12.5///)

```

EACH RESONANCE IS TAKEN SEPERATELY.

```

DO 2 I=1,NR
  IIN=I
  INN=IN
  GAM(I)=GN(I)+GG(I)

```

NECESSARY PARAMETERS FOR RESONANCE INTEGRAL ARE CALCULATED.
(SEE EQ. 3-11)

```

DELTA=(.0186**2)*TEMP*E(I)/A
T=DELTA/(GAM(I)**2)
SGO=2.6E+06*G(I)*GN(I)/(GAM(I)*E(I))
SGOA=SGO*GG(I)/GAM(I)
SGOS=SGO*SGSF*G(I)*GN(I)/GAM(I)
SGOS=SQRT(SGOS)
SGOR=SGOA+SGOS
IF(IWRITE.GT.0) WRITE(6,777) T,DELTA,SGO,SGOA,SGOS
OMEA= W*GAM(I)*SIGAM/(GG(I)*SGO)
OMES= W*GAM(I)*SIGSM/(GN(I)*SGO)
OMEB=WC*SGBAMF*GAM(I)/(GG(I)*SGO)
OMEB= (WC*SGBSMF+SGSF)*GAM(I)/(GN(I)*SGO)
BETA=V*W*SIGRM/SGO
BETAB=(SGSF+WC*SGBRMF)/SGO

```

EYCH0073
EYCH0074
EYCH0075
EYCH0076
EYCH0077
EYCH0078
EYCH0079
EYCH0080
EYCH0081
EYCH0082
EYCH0083
EYCH0084
EYCH0085
EYCH0086
EYCH0087
EYCH0088
EYCH0089
EYCH0090
EYCH0091
EYCH0092
EYCH0093
EYCH0094
EYCH0095
EYCH0096
EYCH0097
EYCH0098
EYCH0099
EYCH0100
EYCH0101
EYCH0102
EYCH0103
EYCH0104
EYCH0105
EYCH0106
EYCH0107
EYCH0108

```

      PHU=SGOS/SGO
      PHUS=PHU*GAM(I)/GN(I)
C
C   CAPTURE CROSS SECTION IS CALCULATED.
C
      OMEX=OMEA
      OMEBX=OMEBA
      PHUX=PHU
      PHUXX=0.0
      POT=0.0
      ZYX(1,K,I)=BETA
      ZYX(2,K,I)=BETAB
      ZYX(3,K,I)=PHU
      IF(IWRITE.GT.0) WRITE(6,3) OMEX,OMEBX,BETA,BETAB,PHUX,PHUXX,POT
C
C   FINE GROUP WIDTH IS DETERMINED SO THAT THE VALUE OF THE RESONANCE
C   INTEGRAL AT THE FINE GROUP BOUNDARY IS 1/100TH OF THE MAX. VALUE.
C
125  XIN=FLOAT(INN)
      SAPSAL=FCT(XIN)/FCT(0.0)-0.01
      IF(SAPSAL) 123,123,124
124  INN=INN+2
      GO TO 125
123  XIN=FLOAT(INN)
      EK(I)=E(I)-XIN*GAM(I)/2.
      EM(I)=E(I)+XIN*GAM(I)/2.
      IF(IWRITE.GT.0) WRITE(6,126) I,EK(I),I,EM(I),INN
      QL=(EK(I)-E(I))/(GAM(I)/2.)
      QU=(EM(I)-E(I))/(GAM(I)/2.)
C
C   INTEGRATION SUBROUTINE IS CALLED.
C
      CALL QAR(FCT,QL,QU,LMN,YINTA,EPS,IERA)
      BABCUM=BETA*BETAB
      RIA=(PI-BABCUM*YINTA)*100./PI
C

```

```

EYCH0109
EYCH0110
EYCH0111
EYCH0112
EYCH0113
EYCH0114
EYCH0115
EYCH0116
EYCH0117
EYCH0118
EYCH0119
EYCH0120
EYCH0121
EYCH0122
EYCH0123
EYCH0124
EYCH0125
EYCH0126
EYCH0127
EYCH0128
EYCH0129
EYCH0130
EYCH0131
EYCH0132
EYCH0133
EYCH0134
EYCH0135
EYCH0136
EYCH0137
EYCH0138
EYCH0139
EYCH0140
EYCH0141
EYCH0142
EYCH0143
EYCH0144

```

```

C      ELASTIC SCATTERING CROSS SECTION IS CALCULATED.
C
OMEX=OMES
OMEBX=OMEBS
PHUX=PHUS
PHUXX=PHUX
POT=SGSF*GAM(I)/(SGO*GN(I))
POT=0.0
IF(IWRITE.GT.0) WRITE(6,3) OMEX,OMEBX,BETA,BETAB,PHUX,PHUXX,POT
CALL QAR(FCT,QL,QU,LMN,YINTS,EPS,IERS)
IF(IWRITE.GT.0) WRITE(6,19) YINTA,YINTS,RIA
C
C      TAIL EFFECTS ARE CALCULATED.
C
DET=BABCUM*(1.+BABCUM)-PHU*PHU
DET=SQRT(ABS(DET))
UL=(EL-E(I))/(GAM(I)/2.)
UU=(EU-E(I))/(GAM(I)/2.)
FIRST=BABCUM*QL+PHU
SECON=BABCUM*QU+PHU
THIRD=BABCUM*UU+PHU
FORTH=BABCUM*UL+PHU
FIRST=FIRST/DET
SECON=SECON/DET
THIRD=THIRD/DET
FORTH=FORTH/DET
FIRST=ATAN(FIRST)
SECON=ATAN(SECON)
THIRD=ATAN(THIRD)
FORTH=ATAN(FORTH)
CORREC= (ABS(FIRST-FORTH)+ABS(SECON-THIRD))/DET
OMO=1.0
COCL=1./(1.+TAUC*QQ/3.)
IF(IRATIO.EQ.1) OMO=0.0
CORR=1.+OMO*COOL*TAUC*(1.-QQ)/3.
IF(IWRITE.GT.0) WRITE(6,25) CORREC,CORR

```

```

EYCH0145
EYCH0146
EYCH0147
EYCH0148
EYCH0149
EYCH0150
EYCH0151
EYCH0152
EYCH0153
EYCH0154
EYCH0155
EYCH0156
EYCH0157
EYCH0158
EYCH0159
EYCH0160
EYCH0161
EYCH0162
EYCH0163
EYCH0164
EYCH0165
EYCH0166
EYCH0167
EYCH0168
EYCH0169
EYCH0170
EYCH0171
EYCH0172
EYCH0173
EYCH0174
EYCH0175
EYCH0176
EYCH0177
EYCH0178
EYCH0179
EYCH0180

```

```

CORREC=CORREC/CORR
IF(EK(I).LE.EL) CORREC=0.0
IF(EM(I).GE.EU) CORREC=0.0
IF(IWRITE.GT.0) WRITE(6,26) CORREC
YINTA=YINTA+CORREC
XXX1=BABCUM*(QL**2)+2.*PHU*QL+BABCUM+1.
XXX2=BABCUM*(QU**2)+2.*PHU*QU+BABCUM+1.
XXX3=BABCUM*(UU**2)+2.*PHU*UU+BABCUM+1.
XXX4=BABCUM*(UL**2)+2.*PHU*UL+BABCUM+1.
XXX1=ALOG(XXX1)
XXX2=ALOG(XXX2)
XXX3=ALOG(XXX3)
XXX4=ALOG(XXX4)
DE=2.*PHU/BABCUM
CORRS=(ABS(XXX1-XXX4)+ABS(XXX2-XXX3))/DE
CORRS=(1.-(2.*PHU**2/BABCUM))*CORREC+CORRS
IF(IWRITE.GT.0) WRITE(6,25) CORRS,CORR
CORRS=CORRS/CORR
IF(EK(I).LE.EL) CORRS=C.0
IF(EM(I).GE.EU) CORRS=0.0
IF(IWRITE.GT.0) WRITE(6,26) CORRS
YINTS=YINTS+CORRS
RIA=(PI-BABCUM*YINTA)*100./PI
IF(IWRITE.GT.0) WRITE(6,19) YINTA,YINTS,RIA
RR(I)=(GG(I)/2.)*((1./E(I))**XN)*YINTA
GGG(I)=(GN(I)/2.)*((1./E(I))**XN)*YINTS
RR(I)=RR(I)/DDD
GGG(I)=GGG(I)/DDD
IF(IWRITE.GT.0) WRITE(6,17) I,RR(I),IERA
IF(IWRITE.GT.0) WRITE(6,18) I,GGG(I),IERS
2 CONTINUE
CALL SUM2(RATT,RATT1,RR,GGG,NR)
RETURN
END

```

```

EYCH0181
EYCH0182
EYCH0183
EYCH0184
EYCH0185
EYCH0186
EYCH0187
EYCH0188
EYCH0189
EYCH0190
EYCH0191
EYCH0192
EYCH0193
EYCH0194
EYCH0195
EYCH0196
EYCH0197
EYCH0198
EYCH0199
EYCH0200
EYCH0201
EYCH0202
EYCH0203
EYCH0204
EYCH0205
EYCH0206
EYCH0207
EYCH0208
EYCH0209
EYCH0210
EYCH0211
EYCH0212
EYCH0213
EYCH0214

```

SUBROUTINE DUZELT(TESIR)

THIS SUBROUTINE CALCULATES THE EFFECTS OF OTHER RESONANCES IN OTHER GROUPS
ON THE BROAD GROUP UNDER CONSIDERATION.
ASSUMES A $1./(1.+X**2)$ TAIL AND CALCULATES THE INTEGRAL USING STANDART
FORMULAS.

REAL MDEN
INTEGER BGG
COMMON/CE/RF,RC,MDEN,PCEN,RDEN,TAUC,TEMP,A
COMMON/CWR/ IWRITE
COMMON/CER/ IBG(13),XEU(13),XEL(13),XNX(13),INR(13),XYZ(4,13,150),
IBGG,ZYX(3,13,150)
COMMON/CC/SIGAM,SIGSM,SGBSMF,SGBAMF,SGAF,SGSF,V,W,WC,RO,XIF,XIM
DIMENSION DELTAU(13),FONK(13,150),FON(13,13),TESIR(13)
EXTERNAL DUZ
EXTERNAL EPART
65 FORMAT(4(2X,'TESIR(',I2,')=',E12.5,' ',''))
DO 1111 L=1,BGG
TESIR(L)=0.0
DO 1111 M=1,BGG
1111 FON(M,L)=0.0
DO 1 I=1,BGG
EU=XEU(I)
EL=XEL(I)
XN=XNX(I)
NR=INR(I)
DELTAU(I)=EPART(EU,EL,XN)
DO 2 J=1,NR
E=1.+(1.+2.*RF*RDEN*XYZ(3,I,J)/(XYZ(2,I,J)+XYZ(3,I,J)))*ZYX(1,I,J)
1+ZYX(2,I,J)
B=2.*ZYX(3,I,J)
C=ZYX(1,I,J)+ZYX(2,I,J)
F=(XYZ(2,I,J)+XYZ(3,I,J))/(XYZ(1,I,J)**XNX(I))

DUZE0001
DUZE0002
DUZE0003
DUZE0004
DUZE0005
DUZE0006
DUZE0007
DUZE0008
DUZE0009
DUZE0010
DUZE0011
DUZE0012
DUZE0013
DUZE0014
DUZE0015
DUZE0016
DUZE0017
DUZE0018
DUZE0019
DUZE0020
DUZE0021
DUZE0022
DUZE0023
DUZE0024
DUZE0025
DUZE0026
DUZE0027
DUZE0028
DUZE0029
DUZE0030
DUZE0031
DUZE0032
DUZE0033
DUZE0034
DUZE0035
DUZE0036

```

F=SGSF*F/2.
DO 23 K=1,BGG
IF(K.EQ.I) GO TO 33
XU=2.*(XEU(K)-XYZ(1,I,J))/(XYZ(2,I,J)+XYZ(3,I,J))
XL=2.*(XEL(K)-XYZ(1,I,J))/(XYZ(2,I,J)+XYZ(3,I,J))
FONK(K,J)=ABS(DUZ(E,B,C,XU)-DUZ(E,B,C,XL))
FONK(K,J)=FONK(K,J)*F/DELTAU(I)
GO TO 23
33 FONK(K,J)=0.0
23 CONTINUE
2 CONTINUE
DO 22 K=1,BGG
DO 21 J=1,NR
IF(K.EQ.I) GO TO 222
FON(K,I)=FON(K,I)+FONK(K,J)
GO TO 21
222 FON(K,I)=0.0
21 CONTINUE
22 CONTINUE
1 CONTINUE
DO 12 K=1,BGG
DO 11 I=1,BGG
11 TESIR(K)=TESIR(K)+FON(K,I)
12 CONTINUE
IF(IWRITE.GT.0) WRITE(6,65) (K, TESIR(K), K=1,BGG)
RETURN
END

```

```

DUZE0037
DUZE0038
DUZE0039
DUZE0040
DUZE0041
DUZE0042
DUZE0043
DUZE0044
DUZE0045
DUZE0046
DUZE0047
DUZE0048
DUZE0049
DUZE0050
DUZE0051
DUZE0052
DUZE0053
DUZE0054
DUZE0055
DUZE0056
DUZE0057
DUZE0058
DUZE0059
DUZE0060
DUZE0061
DUZE0062
DUZE0063

```


SUBROUTINE PSIXI(X,T,U,V)

THIS SUBROUTINE CALCULATES THE VOIGT FUNCTIONS BY USING THE APPROXIMATE
METHOD DEVELOPED BY C.CHIARELLA AND A.REICHEL, **MATH. COMP.** ,V=22,137.
THIS SUBROUTINE IS TAKEN FROM MIGROS-2 ** KFK-1784 **
AN ERROR IN THIS SUBROUTINE WAS FOUND AND CORRECTED.

DIMENSION C(8),D(8)
PI=3.141593
RTPI=SQRT(PI)
H=0.7
CALL EXPPX(C,D,H)
XX=X*X
BB=1.+XX
IF(T.NE.0.0) GO TO 3
U=1./BB
V=U*X
GO TO 2
3 HORP=H/RTPI
U=HORP/BB
V=U*X
DO 1 N=1,8
AA=4.*T*C(N)
CC=2.*HORP*D(N)
ALPHA=1.-XX+AA
DIV=1./((ALPHA*ALPHA+4.*XX)
U=U+CC*(BB+AA)*DIV
1 V=V+CC*X*(BB-AA)*DIV

A CARD WAS REMOVED FROM THE ORIGINAL SUBROUTINE OF MIGROS-2

RT=SQRT(T)
ETA=PI/(H*RT)
EXPO=(XX-1.)/(4.*T)

PSIX0001
PSIX0002
PSIX0003
PSIX0004
PSIX0005
PSIX0006
PSIX0007
PSIX0008
PSIX0009
PSIX0010
PSIX0011
PSIX0012
PSIX0013
PSIX0014
PSIX0015
PSIX0016
PSIX0017
PSIX0018
PSIX0019
PSIX0020
PSIX0021
PSIX0022
PSIX0023
PSIX0024
PSIX0025
PSIX0026
PSIX0027
PSIX0028
PSIX0029
PSIX0030
PSIX0031
PSIX0032
PSIX0033
PSIX0034
PSIX0035
PSIX0036

```

IF(EXPO.GT.25.) GO TO 2
XI=X/(2.*T)
ZETA=X*ETA
ACOS= COS(XI)
BCOS= COS(XI-ZETA)
ASIN= SIN(XI)
BSIN= SIN(XI-ZETA)
BOT=1./((1.-2.* EXP(ETA)* COS(ZETA)+ EXP(2.*ETA))
REAL=BOT*(ACOS- EXP(ETA)*BCOS)
AMAG=BOT*(-ASIN+ EXP(ETA)*BSIN)
EXIT=RTPI* EXP(-EXPO)/RT
U=U+EXIT*REAL
V=V-EXIT*AMAG
2 RETURN
END

```

```

PSIX0037
PSIX0038
PSIX0039
PSIX0040
PSIX0041
PSIX0042
PSIX0043
PSIX0044
PSIX0045
PSIX0046
PSIX0047
PSIX0048
PSIX0049
PSIX0050
PSIX0051

```

SUBROUTINE EXPPX(C,D,H)

THIS SUBROUTINE CALCULATES AN EXPONANTIAL.

DIMENSION C(8),D(8)

DO 1 N=1,8

ENN=N*N

C(N)=ENN*H*H

D(N)= EXP(-C(N))

1 CONTINUE

RETURN

END

EXPP0001
EXPP0002
EXPP0003
EXPP0004
EXPP0005
EXPP0006
EXPP0007
EXPP0008
EXPP0009
EXPP0010
EXPP0011
EXPP0012
EXPP0013
EXPP0014

SUBROUTINE SUM2(RATT,RATT1,RR,GGG,NR)

THIS SUBROUTINE SUMS THE EFFECTS OF EACH RESONANCE CROSS SECTION.

COMMON/CWR/ IWRITE

DIMENSION RR(150),GGG(150)

4 FORMAT(2X,'***** RATT=','E12.5,', RATT1=','E12.5,'*****')

RATT=0.0

RATT1=0.0

DO 3 I=1,NR

RATT=RATT+RR(I)

3 RATT1=RATT1+GGG(I)

IF(IWRITE.GT.0) WRITE(6,4) RATT,RATT1

RETURN

ENC

SUM20001

SUM20002

SUM20003

SUM20004

SUM20005

SUM20006

SUM20007

SUM20008

SUM20009

SUM20010

SUM20011

SUM20012

SUM20013

SUM20014

SUM20015

SUM20016

SUM20017

FUNCTION FCT(Q)

THIS FUNCTION CALCULATES THE INTEGRAND OF THE RESONANCE INTEGRAL FOR
VARIOUS CASES.

C
C
C
C
C
C
COMMON/CFCT/ T,SGO,SGOA,SGOS,OMEX,OMEBX,PHUX,BETA,BETAB,QQ,PHU
1,PHUXX,POT
COMMON/CC/SIGAM,SIGSM,SGBSMF,SGBAMF,SGAF,SGSF,V,W,WC,RO,XIF,XIM
COMMON/CE/RF,RC,MDEN,PCEN,RDEN,TAUC,TEMP,A
COMMON/CR/E(150),GN(150),GG(150),G(150),EK(150),EM(150),BG,EU,EL,
INR,XN,IN
COMMON/CGAM/GAM(150),IIN
COMMON/CRAT/ IRATIO
2 I=IIN
COOL=1./(1.+TAUC*QQ/3.)
CALL PSIXI(Q,T,U,VV)
SIGOA=U*SGOA
SIGOS=SGO*GN(I)*U/GAM(I)+SGOS*VV+SGSF
TAU=2.*RF*RDEN*(SIGOA+SIGOS-SGSF)
OM=(1.+TANH(.1331*TAU))/3.
RATIO=1.+OM*(1.-TAUC*QQ/3.)*TAU*(1.-QQ)
3 UST=U+PHUXX*VV
ALT=U+PHU*VV+BETAB+BETA*RATIO
FCT=UST/ALT
1 RETURN
END

FCT 0001
FCT 0002
FCT 0003
FCT 0004
FCT 0005
FCT 0006
FCT 0007
FCT 0008
FCT 0009
FCT 0010
FCT 0011
FCT 0012
FCT 0013
FCT 0014
FCT 0015
FCT 0016
FCT 0017
FCT 0018
FCT 0019
FCT 0020
FCT 0021
FCT 0022
FCT 0023
FCT 0024
FCT 0025
FCT 0026
FCT 0027
FCT 0028

FUNCTION DUZ(A,B,C,X)

THIS FUNCTION CALCULATES THE NECESSARY FUNCTION IN DUZELT SUBROUTINE.

DELTA=4.*A*C-B*B

IF(DELTA.LT.0.0) GO TO 1

DELTA=SQRT(DELTA)

FUN=(2.*C*X+B)/DELTA

FUN=ATAN(FUN)

DUZ=2.*FUN/DELTA

GO TO 2

1 DELTA=SQRT(ABS(DELTA))

FUN=(2.*C*X+B)/DELTA

FUN=(1./2.)*ALOG((1.+FUN)/(1.-FUN))

DUZ=-2.*FUN/DELTA

2 RETURN

END

DUZ 0001

DUZ 0002

DUZ 0003

DUZ 0004

DUZ 0005

DUZ 0006

DUZ 0007

DUZ 0008

DUZ 0009

DUZ 0010

DUZ 0011

DUZ 0012

DUZ 0013

DUZ 0014

DUZ 0015

DUZ 0016

DUZ 0017

DUZ 0018

DUZ 0019

FUNCTION EPART(EM,EK,XN)

THIS FUNCTION CALCULATES THE GROUP ENERGY OR LETHERGY WIDTH.

IF(XN.GE.1.0) GO TO 1
2 EPART=(EM**(1.-XN)-EK**(1.-XN))/(1.-XN)
GO TO 3
1 EPART=ALOG(EM/EK)
3 RETURN
END

EPAR0001
EPAR0002
EPAR0003
EPAR0004
EPAR0005
EPAR0006
EPAR0007
EPAR0008
EPAR0009
EPAR0010
EPAR0011
EPAR0012

A.5 Typical Input and Output

The following pages contain a sample input/output for one group (Group 21) of the ABBN group structure for U-238. The row output is augmented by some typed-in supplementary remarks. Since CIDI is not a production code, no attempt has been made to incorporate a polished alphanumeric format.

THIS IS A SAMPLE INPUT DECK.

HETEROGENEOUS CROSS SECTIONS FOR METAL FUELED UNIT CELL.

&NACIS NBG=1,BG1=21,BGL=21,IREP=0,IRePA=0,IWRITE=1,IPUNCH=0 &END

&ECE IBC(1)=21,XEU(1)= 10.0,XEL(1)= 4.65,INR(1)= 1,XNX(1)=1.0 &END

0.66700E 01 0.15000E-02 0.25600E-01 0.10000E 01

&MINE MDEN= C.04223,AM=29.778,SGMA(1)=1*.004001,SGMS(1)=1*1.1446,RC=.7322,

RDEN=0.008108,PDEN=0.0,AM1=C.0,A=238.,SGBFA(1)=1*0.0,SGBFS(1)=1*0.0,

SGFA(1)=1*0.0,SGFS(1)=1*8.181,RF=0.3175,

LMN=10,TEMP=300.,IN=10,IRATIO=2,IQ=1 &END

THIS IS A SAMPLE OUTPUT

HETEROGENEOUS UNIT CELL CALCULATION

COOLANT DENSITY= 0.42230E-01

FUEL PIN DENSITY= 0.0

FUEL-PIN ABS. DENSITY= 0.81080E-02

FUEL-PIN RADIUS= 0.31750E+00 UNIT CELL OUTER RADIUS= 0.73220E+00

TEMP= 0.30000E+03

NUMBER OF BROAD GROUPS= 1 FIRST BROAD GROUP= 21 LAST BROAD GROUP= 21

SOURCE RATIO IN THE FUEL ROD= 1

IQ=1 SOURCE RATIO IS CALCULATED, IQ=0 ALL SOURCES ARE IN THE COOLANT

FLUX RATIO= 2(IRATIO=1,HOMOGENEOUS, OTHERS HETEROGENEOUS)

INTEGRATION HALF WIDTH= 10*GAMMA EXPONENT OF 2 FOR THE 'INTEGRATION SUBROUTINE=10

IREP= 0 IREPA= 0

IWRITE= 1(IF 1 PRINTS RESULTS BY RESONANCE, IF NOT PRINTS ONLY THE FINAL RESULTS)

IPUNCH= 0(IF 1 PUNCHES THE FINAL RESULTS)

NC/N28= 0.52084E+01 N/N28= 0.0 SIG-N/RDEN= 0.25834E+02
 VOL. RATIO= 0.43183E+01 COOLANT OPT. THICKNESS= 0.10800E+00
 XIM= 0.65693E-01 XIF= 0.83799E-02

COOLANT ABS.X-SECTION= 0.40010E-02 COOLANT SCAT. X-SECTION= 0.11446E+01
 FUEL-PIN NON-RESON. ABS. X-SECTION= 0.0 FUEL-PIN NON-RESON. SCAT X-SECTION= 0.0
 FUEL-PIN NON-RESON. ABS. X-SECTION FOR ABS.NUC.= 0.0
 FUEL-PIN NON-RESON. SCAT X-SECTION FOR ABS.NUC.= 0.81810E+01

BROAD GROUP= 21, # RES.= 1, XN= 0.10000E+01
 UPPER ENERGY OF THE GROUP= 0.10000E+02, LOWER ENERGY OF THE GROUP= 0.46500E+01

ENERGY	GAMMA-N	GAMMA-G	G
0.66700E+01	0.15000E-02	0.25600E-01	0.10000E+01

N= 3, RO= 0.10121E+01, QQ= 0.38510E-01

T= 0.39606E+01, DELTA= 0.29087E-02, SGO= 0.21576E+05, SGOA= 0.20382E+05,
 SGOS= 0.98844E+02
 BETA= 0.11973E-02, BETAB= 0.37917E-03, PHUX= 0.45812E-02, PHUXX= 0.0
 EK(1)= 0.31199E+01, EM(1)= 0.10220E+02 IN= 262
 BETA= 0.11973E-02, BETAB= 0.37917E-03, PHUX= 0.82767E-01,
 YINTA= 0.73383E+02 YINTS= 0.65113E+02
 % DIFF. FROM ANALYTICAL CROSS SECTION= 0.96317E+02
 YINTA= 0.73383E+02 YINTS= 0.65113E+02
 % DIFF. FROM ANALYTICAL CROSS SECTION= 0.96317E+02
 RR(1)= -0.62392E+01 IER= 0
 GGG(1)= 0.32438E+00 IER= 0

***** RATT= 0.62392E+01, RATT1= 0.32438E+00*****
 DDD= 0.22571E-01

GROUP	SIGMA-ABS.	SIGMA-SCT.	SIGMA-TOT.
21	0.62392E+01	0.85054E+01	0.14745E+02
TESIR(1)= 0.0			
GROUP	SIGMA-ABS.	SIGMA-SCT.	SIGMA-TOT.
21	0.62392E+01	0.85054E+01	0.14745E+02

APPENDIX B

Sample Problem

In this appendix a sample numerical example is given to illustrate the use of the various forms of the equivalence theorem derived in Chapter 4.

The calculations are done for a radial blanket unit cell representative of a UO_2 fueled fast breeder reactor, as shown in Fig. 3.1. The dimensions and properties of the representative cell are listed in Table B.1

Energy group 17 of the Bondarenko set is considered as an example. The self-shielding factors at various degrees of self-shielding are, as tabulated in Ref. (B2):

$$f(0) = 0.049$$

$$f(10) = 0.063$$

$$f(100) = 0.13$$

$$f(\infty) = 1.0$$

Using Equation (2-32) to curve fit f vs. σ_0 , and solving for the coefficients, we obtain:

$$A = 0.4755$$

$$B = 0.3972$$

$$C = -7.5936$$

$$D = 0.5245$$

TABLE B.1

UO₂ Fueled Unit Cell ParametersItem

- 1 The fuel pin radius, $r_f = 0.5461$ cm
- 2 Cylindricized unit cell outer radius, $r_c = 0.8978$ cm
- 3 Volume fraction of fuel region, $v_f = 0.37$
- 4 Volume fraction of coolant region, $v_c = 0.63$
- 5 Dirac chord length of fuel pin, $\bar{l}_f = 4V/S = 1.092$ cm
- 6 Dirac chord length of coolant, $\bar{l}_c = 4V/S = 1.86$ cm
- 7 Coolant region (homogenized sodium and steel clad)
density, $N_c = 0.02594$ nuclei/barn cm; fuel region
homogenized UO₂ density, $N_u = 0.0219$
- 8 Coolant removal (absorption plus scattering $\sigma_{ac} + \sigma_{sc} =$
 $3.5879 + 0.006514$) cross section (homogenized value of
macroscopic scattering cross section + N_c), $\sigma_{Rc} = 3.5944$
- 9 Macroscopic scattering cross section of the fuel pin,
(homogenized over the pin volume), $\Sigma_{sf} = N_u \sigma_{pa} + 2N_u \sigma_{sO_2}$
 $= (0.0219)(8.181) + 2(0.0219)(3.31) = 0.3241$
(see item 14 for σ_{pa})
- 10 Optical thickness of the coolant: $\tau_c = N_c \sigma_{Rc} \bar{l}_c = 0.1734$
- 11 Average (elastic) lethargy gain in fuel
 $\xi_{UO_2} = \frac{\xi_u N_u \sigma_{pa} + 2\xi_{O_2} N_u \sigma_{sO_2}}{\Sigma_{sf}} = 0.0567$
- 12 Average lethargy gain in coolant region, (homogenized
coolant and clad), $\xi_c = 0.0529$

- 13 Fraction of the source in the fuel pin (using items 3, 4, 7, 8, 9, 11, 12, Eq. (4-47), and $\Sigma_{sc} = N_c \sigma_{sc}$:
 $Q_f = 0.4417$; hence $Q_c = (1 - Q_f) = 0.5583$
- 14 Potential scattering cross section of the resonance absorber,
 $\sigma_{pa} = 8.181$ barn. Eg: use $\sigma_{pa} = 4\pi R^2$ where R is the radius of the absorber nucleus.
- 15 Total non-resonant macroscopic cross section of the cell,
 (homogenized over the cell volume),
 $\Sigma_T = N_c v_c \sigma_{Rc} + [\Sigma_{sf} - N_o \sigma_{pa}] v_f = 0.2094$
- 16 Resonance absorber density, (homogenized over the cell volume),
 $N_o = \Sigma_T / N_u = 0.008108$
- 17 Background cross section per absorber nucleus,
 $\sigma_o = \Sigma_T / N_o = 25.836$ barns

The modified background cross section σ_o' is calculated by

$$\sigma_o' = \frac{\sigma_o + \sigma_{pa}}{1 + \tau_c Q_c / 3} - \sigma_{pa} \quad \text{B.1}$$

Using items 10, 13, 14 and 17 from Table B.1

$$\sigma_o' = 24.774 \text{ barn}$$

Using Equation (2-32) along with the above calculated coefficients

A, B, C, D, the interpolated values of f at σ_o and σ_o' are:

$$f_{\text{hom}}(\sigma_o) = 0.07829$$

$$f_{\text{hom}}(\sigma_o') = 0.07736$$

The ratio of the heterogeneous and homogeneous self-shielding factors is:

$$\frac{f_{\text{het}}(\sigma_o)}{f_{\text{hom}}(\sigma_o)} = \frac{f_{\text{het}}(\sigma_o')}{f_{\text{hom}}(\sigma_o')} = 0.988$$

which is in very good agreement with the CIDI results, for the 102.6 eV resonance (which falls within Bondarenko Group 17) as tabulated in

Table 4.2. The approximate relation, Equation (4-43), with

$Q_c = 0.5583$, $f_{\text{hom}}(\sigma_o) = 0.07829$ and $\tau_c = 0.1734$ yields

$$\frac{f_{\text{het}}(\sigma_o)}{f_{\text{hom}}(\sigma_o)} = 0.984$$

APPENDIX C

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