Overview of The WIMS 9 Resonance Treatment

A Report produced for ANSWERS

D J Powney
T D Newton

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Serco Assurance
D J Powney
Winfrith Technology Centre
Dorchester
Dorset
DT2 8ZE
Telephone: +44 (0)1305 851201
Facsimile: +44 (0)1305 851105
E-mail: dave.powney@sercoassurance.com

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	Name	**Signature**	**Date**
Author	D J Powney		
Reviewed by	J L Hutton		
Approved by	T D Newton		

Executive Summary

This report is an overview of the physics methods employed in the resonance treatment in WIMS9. The report demonstrates how more complex problems in neutron slowing down can be related to a simple calculation comprising a resonant nuclide and a hydrogen like scatterer. Two methods of performing the resonance calculation, equivalence theory and subgroup theory are discussed. The full theory involves a series of lengthy algebraic derivations. This report describes the methods in a level of detail such that the WIMS9 user can gain an appreciation of the assumptions made in the derivation, and hence the range of applicability of the methods, without having to follow the complete derivation.

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1 Introduction

WIMS (Winfrith Improved Multigroup Scheme) is a deterministic neutron transport code, not subject to the statistical uncertainties of Monte Carlo. WIMS calculates neutron flux distributions and values of k-infinity or k-effective for an extensive range of reactor cell types. To carry out the calculation it has to solve a mathematical form of the neutron transport equation and some approximations are required in order to solve the equations efficiently.

The most important of the approximations is the use of energy groups. Neutron cross sections are complicated functions of energy and it is necessary to average them in some way over discrete energy ranges. This process is performed prior to the start of a WIMS calculation and results in a nuclear data library which is read from but never written to by WIMS. The averaging is performed so that the reaction rate in a given energy range or group is preserved, because the solution is a function of reaction rates. The mean cross section for reaction x within a group is therefore given by.

$$\overline{\sigma}_x = \frac{\int_{u_l}^{u_u} \sigma_x(u)\phi(u)du}{\int_{u_l}^{u_u} \phi(u)du}$$

Where u_l and u_u are the lower and upper lethargies of the group respectively.

As the flux for a given problem is not known at the library generation stage an assumption about the flux must be used in the library production process.

For cross sections which only vary slowly with lethargy sufficient accuracy is obtained by using a fixed functional form for the flux. In WIMS9 the total energy space is divided into 3 regions:

- Fast region 20MeV to 183.2 keV
- Resonance region 183.2 keV to 4eV
- Thermal region below 4 eV

In the fast region, the fixed form for the flux is the U^{235} fission spectrum; in the resonance region, the flux varies as 1/E (constant in lethargy); in the thermal region, the flux employed is a Maxwellian distribution.

For cross sections which exhibit resonance type behaviour the cross sections can change by many orders of magnitude. In this situation, the flux is strongly dependent on the particular problem and the assumption of a fixed functional form is not adequate. In order to produce a library which can be used on any thermal reactor, cross sections are generated for a number of different forms for the flux. This is carried out by solving the neutron slowing down equations for a simple homogeneous mixture of a single resonance isotope and a fictitious nuclide which has the scattering properties of hydrogen. For WIMS9 the slowing down equations are solved by the NJOY code. By varying the ratio of the resonance absorbing isotope to the scattering isotope the amount of flux depression at the resonance energies varies, giving different values for the group averaged cross sections. These tabulated values are used in the treatment of resonance shielding.

The essence of the resonance treatments in WIMS9 is to relate more complex problems, in particular heterogeneous problems containing mixtures of resonance and moderating nuclides, to the homogeneous data stored in the WIMS library. There are two methods of calculating resonance shielding effects in WIMS9: equivalence theory and subgroup theory. Equivalence theory for both homogeneous and heterogeneous geometries is implemented in the HEAD module. Sub-group theory is implemented by following the calculation of HEAD by the module PRES, a collision probability theory module and then the module RES. Optionally, the collision probability module can be replaced by a run of the CACTUS flux module. This option is automatically detected and the CACTUS flux is used in place of the flux solution performed by RES using the calculated collision probabilities.

The HEAD module calculates absorption, scatter, fission and broad group removal cross-sections for the resonance nuclides.

In HEAD a fine energy group calculation is performed for three purposes:

- To calculate a correction to the broad group outscatter cross section due to the perturbation of the flux by the resonance nuclides.
- To generate a current spectrum which is used to form current weighted transport cross sections.
- To evaluate the interaction effects betweeen the resonances of the different nuclides.

In the high energy part in the resonance region a statistical overlap interaction model between resonances is sufficiently accurate. For energies from 4eV to 52eV, the resonances are broad enough that the use of 100 fine groups, of equal energy width, can model them sufficiently well. Both methods suffer some inaccuracy at mid range resonance energies and for these groups the statistical overlap model is employed. HEAD, as well as applying these corrections to its output equivalence theory broad group cross-sections, also outputs these corrections in the form of correction factors for application in sub-group theory calculations.

The convention used in this report to denote cross-sections and fluxes, unless otherwise stated is:

$\sigma(u)$ = lethargy dependent microscopic cross-section.

$\overline{\sigma}$ = broad group average microscopic cross-section.

$\hat{\sigma}(u)$ = lethargy dependent macroscopic cross-section due to all nuclides except the one of immediate interest divided by the nuclide number density of the nuclide of immediate interest (the background cross-section).

$\hat{\sigma}$ = group average background macroscopic cross-section.

$\Sigma(u)$ = lethargy dependent macroscopic cross-section.

$\overline{\Sigma}$ = group average macroscopic cross-section.

$\phi(u)$ = lethargy dependent neutron flux.

$\overline{\phi}$ = group average neutron flux.

2 Neutron Slowing Down

The slowing down of fast neutrons in the resonance region is due almost entirely to elastic scattering suffered by the neutrons with the nuclei of the moderator. Experiments indicate that the elastic scattering of neutrons with energies of less than a few MeV is isotropic in the centre of mass frame. The assumptions of elastic (i.e. no change in the internal energy of the target nucleus) and isotropic scattering enable us to apply classical mechanics to the slowing down process and derive approximate formulae for neutron reaction rates, which we can in turn relate back to the exact solution of the slowing down equations performed in NJOY.

By applying the principles of conservation of momentum and energy to the neutron and target before and after a scattering collision the final energy E_2 can be expressed in terms of the initial energy E_1 and the angle of scatter in the centre of mass frame θ [1].

$$\frac{E_2}{E_1} = \frac{1}{2}\left[(1+\alpha)+(1-\alpha)\cos\theta\right]$$

Where

$$\alpha = \left(\frac{A-1}{A+1} \right)^2$$

A being the atomic mass of the target nucleus.

Taking account the assumption that the scattering is isotropic in the centre of mass frame we can eliminate the angular dependence to obtain $p(E_2)dE_2$, the probability that the final neutron energy lies in the range $E_2 \rightarrow E_2 + dE_2$:

$$p(E_1 \rightarrow E_2)dE_2 = \frac{-dE_2}{E_1(1-\alpha)}$$

It should be observed that this probability is independent of the final energy E2, and that if $\alpha > 0$, which is the situation for all target nuclei except hydrogen, not all of the neutron energy can be lost; the maximum energy loss per collision is $E_1(1-\alpha)$; for hydrogen all of the neutron energy may be lost in a single collision, assuming equal neutron and proton masses.

In neutron slowing down theory is has been found to be more convenient to use the lethargy variable u defined by:

$$u = \ln \frac{E_0}{E}$$

where E is the energy of the neutron and E_0 is a reference energy. The expressions for probability of energy loss and for maximum energy loss can be rewritten in terms of lethargy as:

$$P(u_1 \rightarrow u_2)du_2 = \frac{e^{(u_1 - u_2)}du_2}{1-\alpha}$$

$$\Delta u^{max} = -\ln \alpha$$

Note that a loss of energy corresponds to a gain in lethargy.

3 Homogeneous Resonance Theory

3.1 Group Averaged Cross Sections

Approximations to the nuclide reaction rates calculated in NJOY can be obtained by equating the neutron collision rate to the neutron slowing down density and using the above expression for the probability of scattering to a higher lethargy [1].

$$\Sigma_t(u)\phi(u) = q(u)$$

$\Sigma_t(u)$ = the macroscopic total cross-section.
$\phi(u)$ = flux.
q(u) = the neutron slowing down density.

In the narrow resonance approximation, the average logarithmic energy loss per collision is assumed much larger than the width of the resonances. In this case the contribution to the slowing down density from integration over the resonances can be neglected. The scattering cross-section outside the

resonances is approximately constant and equal to the potential scatter cross-section. The slowing down density is given by:

$$q(u) = \frac{\Sigma_{pot}}{\overline{\xi}}$$

Σ_{pot} = the macroscopic potential scatter cross-section.

$\overline{\xi}$ = the system average logarithmic energy decrement per collision.

In the wide resonance approximation any logarithmic energy loss in a collision is assumed negligible relative to the width of the resonance. All scatter is effectively self scatter neither adding nor removing neutrons. In this case the slowing down density is simply given by the scattering rate:

$$q(u) = \Sigma_s(u)\phi(u)$$

Σ_s = the macroscopic scatter cross-section.

For light nuclei the narrow resonance approximation holds well. For heavy nuclei whether the narrow resonance approximation or the wide resonance approximation is appropriate depends on the individual characteristics of the resonance. Generally, the narrow resonance approximation holds at high resonance energies where resonances tend to be narrow and close together and there is a tendency toward the wide resonance approximation at lower resonance energies where resonances are wide and well separated.

In practice, a mixture of the narrow and wide resonance approximations is needed. This is achieved by using the intermediate resonance approximation proposed by Goldstein and Cohen [2]. The intermediate resonance parameter λ is introduced such that if λ = 1 the narrow resonance approximation results and for λ = 0 the wide resonance approximation applies. This gives the general slowing down density as:

$$q(u) = \frac{\lambda\Sigma_{pot}}{\overline{\xi}} + (1-\lambda)\Sigma_s(u)\phi(u)$$

Equating this to the collision rate per unit lethargy, in a homogeneous geometry with only a single spatial region, gives:

$$\Sigma_t(u)\phi(u) = \frac{\lambda\Sigma_{pot}}{\overline{\xi}} + (1-\lambda)\Sigma_s(u)\phi(u)$$

As the total cross-section is just the sum of the absorption and scatter cross-sections this can be re-arranged to give:

$$\phi(u) = \frac{\lambda\Sigma_{pot}}{\overline{\xi}(\lambda\Sigma_s(u) + \Sigma_a(u))}$$

Introducing a resonance scatter cross-section, which is zero in the absence of resonance scatter, defined as:

$$\Sigma_{rs}(u) = \lambda(\Sigma_s(u) - \Sigma_{pot}) \text{ also define } \Sigma_p = \lambda\Sigma_{pot}$$

Gives:

$$\phi(u) = \frac{\Sigma_p}{\overline{\xi}(\Sigma_p + \Sigma_{rs}(u) + \Sigma_a(u))}$$

At lethargies higher than the resonance lethargy the flux will be reduced due to captures in the resonance. This has an effect on the outscatter cross sections for the higher mass nuclides. A correction to the outscatter cross sections is included in WIMS, based on either a fine group calculation or an evaluation of the resonance escape probability.

We also define:

$$\Sigma_a(u) = \sum_i N_i \sigma_a^i(u) \qquad \lambda = \frac{\sum_i N_i \lambda_i \sigma_s^i(u)}{\sum_i N_i \sigma_s^i(u)} \qquad \Sigma_p = \sum_i N_i \lambda_i \sigma_{pot}^i \qquad \bar{\xi} = \frac{\sum_i N_i \xi_i \sigma_s^i(u)}{\sum_i N_i \sigma_s^i(u)}$$

$$\text{also } \sigma_{rs}^i(u) = \lambda_i(\sigma_s^i(u) - \sigma_{pot}^i) \text{ and } \Sigma_{rs}(u) = \sum_i N_i \lambda_i (\sigma_s^i(u) - \sigma_{pot}^i)$$

$$\sigma_p^i = \frac{\Sigma_p}{N_i}$$

For a single resonance nuclide the broad group average flux can be derived as follows:

$$\bar{\phi} = \int \phi(u)du = \int \frac{\Sigma_p}{\bar{\xi}(\Sigma_p + \Sigma_{rs}(u) + \Sigma_a(u))} du$$

Dividing by the number density of the resonance nuclide and substituting the above expressions for macroscopic cross section we obtain:

$$\bar{\phi} = \frac{1}{\bar{\xi}} \int \frac{\sigma_p^i(u)}{(\sigma_p^i + \sigma_{rs}^i(u) + \sigma_a^i(u))} du$$

Rearranging by adding and subtracting $\sigma_{rs}^i + \sigma_a^i$ to the numerator of the integrand the broad group flux can be related to the resonance integrals stored on the library.

$$\bar{\phi} = \frac{1}{\bar{\xi}} \left[\int du - \int \frac{\sigma_{rs}^i(u) + \sigma_a^i(u)}{(\sigma_p^i + \sigma_{rs}^i(u) + \sigma_a^i(u))} du \right]$$

The library tabulation of resonance integrals for nuclide i, per unit lethargy, for absorption and scatter as a function of both temperature and the amount of scattering per atom of nuclide i are defined to be:

$$I_a^i(\sigma_p) = \frac{1}{\delta u} \int \frac{\sigma_a(u)\sigma_p}{\sigma_p + \sigma_{rs}(u) + \sigma_a(u)} du$$

and

$$I_{rs}^i(\sigma_p) = \frac{1}{\delta u} \int \frac{\sigma_{rs}(u)\sigma_p}{\sigma_p + \sigma_{rs}(u) + \sigma_a(u)} du$$

Noting that σ_p is assumed to be lethargy independent we derive:

$$\bar{\phi} = \frac{\delta u}{\bar{\xi}} \left[1 - \left[\frac{I_{rs}^i(\sigma_p^i)}{\sigma_p^i} + \frac{I_a^i(\sigma_p^i)}{\sigma_p^i} \right] \right]$$

The microscopic broad group average cross-section for nuclide i resonance reaction x is given by:

$$\overline{\sigma}_x^i = \frac{\int \sigma_x^i(u)\phi(u)du}{\int \phi(u)du}$$

Assuming the form of the flux from above then:

$$\overline{\phi}.\overline{\sigma}_x^i = \int \frac{\sigma_x^i(u)\Sigma_p}{\overline{\xi}(\Sigma_p + \Sigma_{rs}(u) + \Sigma_a(u))}du$$

Following a procedure similar to that for the broad group average flux gives:

$$\sigma_x^i = \frac{I_x^i\left(\sigma_p^i\right)}{1 - \left[\frac{I_{rs}^i\left(\sigma_p^i\right)}{\sigma_p^i} + \frac{I_a^i\left(\sigma_p^i\right)}{\sigma_p^i}\right]}$$

In practice, there is an interaction effect between the different resonance nuclides in the problem. The flux depression caused by one nuclide can affect the resonance shielding of another nuclide. In WIMS9 two models are used to treat this problem. In the higher energy part of the resonance region (183.3 keV to 51.6 eV) there are many narrow resonances. Here the resonances are assumed to interact in a random manner, and the expressions for the flux derived above are modified to take into account the contribution to the flux depression from the other nuclides. In the lower energy portion of the resonance region (51.6eV to 4eV), a detailed slowing down calculation is performed within WIMS9. This slowing down calculation generates correction factors defined as:

- (Interacted cross section)/(un-interacted cross section)

These correction factors are used to model the interaction between the various nuclides in the calculation.

Outscatter or removal from a broad group is affected by the presence of resonances within the group. Heavier nuclides may only be able to scatter neutrons out of the broad group from the higher lethargies of the group where the flux may be depressed or enhanced by resonances . In the higher energy region as described above, a correction for this effect is calculated on a nuclide by nuclide basis. This requires the calculation of the resonance escape probability p, and is known as the f(p) factor.

In the lower energy region the fine group calculation is again used to calculate the effect. The correction factors are defined as the ratio of the best estimate result taken from the fine group calculation, to a calculation which represents the NJOY treatment used to generate the library data.

Therefore for resonance nuclides the f(p) correction is defined as:

$$\frac{\left(\text{broad group average removal cross\_section in the presence of all nuclides}\right)}{\left(\text{broad group average removal cross\_section in the absence of all other resonant nuclides}\right)}$$

To derive the f(p) correction for the non-resonant nuclides an additional calculation is carried out in the absence of all absorption which gives the f(p) correction as:

$$\frac{\left(\text{broad group average removal cross\_section in the presence of all nuclides}\right)}{\left(\text{broad group average removal cross\_section in the absence of all absorption}\right)}$$

3.2 Nuclear Data Library from NJOY

The resonance integrals and other quantities needed to evaluate the effective broad group average cross-sections using the formulae developed in the previous sections are read by WIMS from a nuclear data library generated using the NJOY code.

In this context, NJOY solves the neutron slowing down equation for a simple homogeneous mixture of a single resonance absorbing isotope and a fictitious nuclide which has the scattering properties of hydrogen. The NJOY solution is in essence a continuous energy solution which can be used to average cross-sections or resonance integrals over a broad group energy structure specified by the user. Each execution of NJOY provides energy group data for a specific isotope, temperature and ratio of the resonance absorbing isotope to the fictitious hydrogen like scattering nuclide (sigmap value). The nuclear data library is therefore assembled from many executions of the NJOY code to give a full temperature and sigmap parameterisation. In the case of non-resonant nuclides, with no temperature dependent thermal cross-sections, only a single execution of NJOY is required in which the flux is assumed to have the shape of the fission spectrum at high energy, to be of the form 1/energy in the resonance range and to have a Maxwellian thermal energy dependence.

The ratio of the resonance isotope to the fictitious hydrogen like scattering nuclide, the sigmap value, is given in the input to NJOY by specifying the energy independent potential scattering cross-section due to the fictitious nuclide σ_0. NJOY takes the number density of the resonance nuclide to be unity and therefore the potential scattering cross-section in the calculation, per atom of resonance isotope, is:

$$\sigma_p^i = \sigma_0 + \lambda_i \sigma_{pot}^i$$

The definition of the potential scattering, per atom of the resonant isotope, in a homogeneous mixture of the resonance isotope and hydrogen, is given by:

$$\sigma_p^i = \frac{N_H}{N_i}\sigma_{pot}^H + \lambda_i \sigma_{pot}^i$$

Comparison of the above equations shows that the input value of σ_0 specifies the ratio of the hydrogen like nuclide to the resonant isotope.

WIMS 9 takes resonance integrals from NJOY for four reactions, absorption, fission, resonance scatter and removal. These integrals are formed from the broad group average cross-sections derived in the NJOY execution:

$$I_a^i(\sigma_p) = \frac{1}{\delta u}\int \frac{\sigma_a^i(u)\sigma_p}{\sigma_p + \sigma_{rs}^i(u) + \sigma_a^i(u)}\,du = \frac{\overline{\sigma}_a^i \sigma_p}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i}$$

$$I_f^i(\sigma_p) = \frac{1}{\delta u}\int \frac{\sigma_f^i(u)\sigma_p}{\sigma_p + \sigma_{rs}^i(u) + \sigma_a^i(u)}\,du = \frac{\overline{\sigma}_f^i \sigma_p}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i}$$

$$I_{rs}^i(\sigma_p) = \frac{1}{\delta u}\int \frac{\sigma_{rs}^i(u)\sigma_p}{\sigma_p + \sigma_{rs}^i(u) + \sigma_a^i(u)}\,du = \frac{\overline{\sigma}_{rs}^i \sigma_p}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i}$$

$$I_r^i(\sigma_p) = \frac{1}{\delta u}\int \frac{\sigma_r^i(u)\sigma_p}{\sigma_p + \sigma_{rs}^i(u) + \sigma_a^i(u)}\,du = \frac{\overline{\sigma}_r^i \sigma_p}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i}$$

It is re-called that the definition of the resonance scattering cross-section is:

$$\sigma_{rs}^i(u) = \lambda_i(\sigma_s^i(u) - \sigma_{pot}^i)$$

The bar above the cross-section denotes the group average value. If a simple mixture of a resonance isotope and hydrogen is considered then it can be verified that the use of these definitions, when substituted into the equation for the broad group average cross-section given in Section 3.1, exactly recovers the NJOY broad group average cross-section. For example to recover the group averaged absorption cross section we proceed as follows:

$$\frac{1}{\sigma_p}\left(I_a^i + I_{rs}^i\right) = \frac{\overline{\sigma}_a^i + \overline{\sigma}_{rs}^i}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i}$$

$$1 - \frac{1}{\sigma_p}\left(I_a^i + I_{rs}^i\right) = \frac{\sigma_p}{\sigma_p + \overline{\sigma}_{rs}^i + \overline{\sigma}_a^i} = \frac{I_a^i}{\overline{\sigma}_a^i}$$

Which gives

$$\overline{\sigma}_a^i = \frac{I_a^i}{1 - \frac{1}{\sigma_p}\left(I_a^i + I_{rs}^i\right)}$$

as required.

4 Equivalence Theory

4.1 Equivalence Relation

The purpose of the equivalence treatment is to form a relationship between heterogeneous geometry and homogeneous geometry problems. The heterogeneous problem can then be solved by the solution of one or more homogeneous problems. The effect of the heterogeneous geometry is to provide additional paths for neutrons, outside the fuel, to avoid collisions in the fuel resonances and thereby act as an effective increase in the neutron scattering cross-section relative to a homogeneous geometry. The heterogeneous system is approximated by a two region system consisting of a region containing resonance nuclides, denoted f, and a region containing moderator, denoted m. The neutron balance for the system can be written as:

$$\Sigma_t^f(u) V_f \phi_f(u) = \psi_f(u) V_f P_{ff} + \psi_m(u) V_m P_{mf}$$

where:
$\phi_f(u)$ = fuel flux
$\Sigma_t^f(u)$ = fuel total cross-section
V_f = fuel volume
$\psi_f(u)$ = the slowing down density in the fuel
P_{ff} = fuel to fuel first flight collision probability
V_m = moderator volume
$\psi_m(u)$ = slowing down density in the moderator
P_{mf} = moderator to fuel first flight collision probability

In the fuel region the intermediate resonance approximation is used for the slowing down density. This approximation is a mixture of the narrow resonance approximation in which neutrons are assumed to suffer an energy loss per scattering collision much greater than the width of the resonance and the wide resonance approximation in which neutrons are assumed to suffer a negligible energy loss per scattering collision. In the narrow resonance approximation the contribution to the slowing down density from integration over the resonance is neglected. Outside the resonances the scatter cross-section is assumed constant and can be replaced by the potential scattering cross-section. The flux

solution for this problem is a constant and assuming a normalisation of the flux to unity, the slowing down density is simply given by:

$$\psi(u) = \Sigma_{pot}$$

In the wide resonance approximation there is no energy loss in a scattering event, all scatter is assumed self scatter, the slowing down density is constant and:

$$\psi(u) = \Sigma_s(u)\phi(u)$$

The intermediate resonance approximation combines these two approximations using the Goldstein and Cohen intermediate resonance parameter λ to give the slowing down density in the fuel as:

$$\psi_f(u) = \lambda\Sigma^f_{pot} + (1-\lambda)\Sigma^f_s(u)\phi(u)$$

In the moderator there are no resonances and the narrow resonance approximation is used. Also the absorption in the moderator is negligible and the potential scatter cross-section can be replaced by the total cross-section:

$$\psi_m(u) = \Sigma^m_t(u)$$

This gives:

$$(\Sigma^f_t(u) - P_{ff}(1-\lambda)\Sigma^f_s(u))V_f\phi_f(u) = \lambda\Sigma^f_{pot}V_fP_{ff} + V_mP_{mf}\Sigma^m_t(u)$$

The region-wise flat flux approximation is used to relate the 'moderator to fuel' first flight collision probability to the 'fuel to fuel' first flight collision probability. From reciprocity:

$$V_mP_{mf}\Sigma^m_t(u) = V_f\Sigma^f_t(u)P_{fm}$$

Also, given that all neutrons collide in the system:

$$P_{fm} + P_{ff} = 1$$

Therefore:

$$(\Sigma^f_t(u) - P_{ff}(1-\lambda)\Sigma^f_s(u))\phi_f(u) = \lambda\Sigma^f_{pot}P_{ff} + \Sigma^f_t(u)(1-P_{ff})$$

The rational approximation, first introduced by Wigner, is now introduced for the form of the fuel to fuel first flight collision probability:

$$P_{ff} = \frac{\Sigma^f_t(u)}{\Sigma^f_t(u) + \Sigma_e} \quad \text{where} \quad \Sigma_e = \frac{S_f}{4V_f} = (\text{mean\_cord})^{-1}$$

Substitution gives:

$$\phi_f(u) = \frac{(\Sigma^f_p + \Sigma_e)}{(\Sigma^f_p + \Sigma_e) + \Sigma^f_{rs}(u) + \Sigma^f_a(u)}$$

in which the following relations have been used:

$$\Sigma^f_t(u) = \Sigma^f_a(u) + \Sigma^f_s(u) \quad \text{and} \quad \lambda\Sigma^f_{pot} = \Sigma^f_p \quad \text{and} \quad \lambda\Sigma^f_s(u) = \Sigma^f_{rs}(u) + \Sigma^f_p$$

This form for the flux is the same as that found for homogeneous geometry but with the potential scatter cross-section enhanced by the escape cross-section. The equivalence relation has been established:

In the case where the total fuel to fuel first flight collision probability can be expressed in single rational form, the heterogeneous geometry can be represented by an equivalent homogeneous geometry in which the potential scattering cross-section is augmented by the escape cross-section.

The single rational approximation to the fuel to fuel first flight collision probability can be improved by the introduction of the bell factor a, such that:

$$P_{ff} = \frac{\Sigma_t^f(u)}{\Sigma_t^f(u) + a\Sigma_e}$$

It is also sometimes useful to employ a double rational approximation to the fuel to fuel first flight collision probability of the form:

$$P_{ff} = \frac{\beta\Sigma_t^f(u)}{\Sigma_t^f(u) + \alpha_1\Sigma_e} + \frac{(1-\beta)\Sigma_t^f(u)}{\Sigma_t^f(u) + \alpha_2\Sigma_e}$$

In this case a strict equivalence relation can not be derived. However, this approximation is not too gross if this relation is only used to establish the multi-term equivalence between the heterogeneous and homogeneous systems. In this case the flux is assumed to be of the form:

$$\phi_f = \sum_j \frac{\beta_j(\Sigma_p^f + \alpha_j\Sigma_e)}{(\Sigma_p^f + \alpha_j\Sigma_e) + \Sigma_{rs}^f(u) + \Sigma_a^f(u)}$$

The full equivalence relation can be stated as

In the case where the total fuel to fuel first flight collision probability can be expressed as the sum of rational expressions, the heterogeneous geometry can be represented by the sum of a set of weighted homogeneous geometries, weights β_j in which the potential scattering cross-section is augmented respectively by $\alpha_j\Sigma_e$.

Mathematically the heterogeneous resonance integral is given by:

$$I_x^i(het) = \sum_j \beta_j I_x^i\left(\frac{\Sigma_p + \alpha_j\Sigma_e}{N_i\psi_i}\right)$$

4.2 Infinite Cell Arrays

The objective here is to evaluate the heterogeneous value of sigmap to use in the evaluation of the homogeneous equivalent resonance integrals for an array of pin cells. From before:

$$\Sigma_p^{het} = \Sigma_p + \alpha\Sigma_e \quad \text{where} \quad \Sigma_p = \sum_i N_i\sigma_p^i \quad \text{and} \quad \Sigma_e = \frac{S_f}{4V_f}$$

V_f = fuel volume.
S_f = fuel surface area.
N_i = nuclide volume density for nuclide i in the fuel region.
σ_i = microscopic potential scatter of nuclide i.

The unknown value is alpha which originates in the expression for the system fuel to fuel first flight collision probability which in terms of broad group average values is given by:

$$P = \frac{\Sigma_t^f}{\Sigma_t^f + \alpha\Sigma_e}$$

To derive alpha for an infinite array of cells an average unit cell, as defined in the last section, is considered which consists of a fuel region (f) and a series of non-fuelled regions (j) and has an outer surface S_b. The following first flight probabilities are defined for the average cell:

p_{ff} = the probability of neutrons born uniformly and isotropically in the fuel to suffer their first collision in the fuel;

p_{fb} = probability of those neutrons to reach the cell boundary S_b uncollided;

p_{bf} = probability of neutrons entering the cell through S_b, with a cosine distribution with respect to the normal on S_b, to suffer their first collision in the fuel;

p_{bb} = probability of those neutrons to traverse the cell uncollided.

Define the transmission probabilities as:

t_{fb} = the probability of neutrons leaving the surface of the fuel S_f with a cosine distribution, to reach S_b uncollided.

t_{bf} = the probability of neutrons entering with a cosine distribution through S_b to reach S_f uncollided.

From these average cell probabilities the system fuel self-collision probability, of an infinite array of pins, can be defined by following neutrons from cell to cell until they collide:

$$P = p_{ff} + p_{fb}p_{bf} + p_{fb}p_{bb}p_{bf} + p_{fb}p_{bb}p_{bb}p_{bf} + ...$$

giving:

$$P = p_{ff} + \frac{p_{fb}p_{bf}}{(1-p_{bb})}$$

from reciprocity:

$$p_{bf} = \frac{4V_f\Sigma_t^f}{S_b}p_{fb}$$

Regardless of the number of regions between S_f and S_b:

$$p_{fb} = t_{fb}(1-p_{ff})$$

Therefore:

$$P = p_{ff} + \frac{\frac{S_f\Sigma_t^f}{S_b\Sigma_e}t_{fb}^2(1-p_{ff})^2}{(1-p_{bb})}$$

To proceed further an expression is needed for the first flight cell blackness ($1-p_{bb}$). This can be calculated from its three contributions:

- Collisions of neutrons that have never reached the fuel $= \sum_{j\neq f} p_{bj}$.
- collisions inside the fuel $= t_{bf}\gamma_f$ where gamma is the fuel first flight blackness.
- Collisions of neutrons that have traversed the fuel $= t_{bf}(1-\gamma_f)(1-t_{fb})$

Using the reciprocity relation $S_f t_{fb} = S_b t_{bf}$ and that:

$$\gamma_f = \frac{4V_f \Sigma_t^f}{S_f}(1-p_{ff}) = \frac{\Sigma_t^f}{\Sigma_e}(1-p_{ff})$$

Gives:

$$(1-p_{bb}) = \frac{S_f \Sigma_t^f}{S_b \Sigma_e} t_{fb}^2 (1-p_{ff}) + \sum_{j \neq f} p_{bj} + t_{bf}(1-t_{fb})$$

therefore:

$$P = p_{ff} + \frac{\Sigma_t^f (1-p_{ff})^2}{\Sigma_t^f (1-p_{ff}) + \frac{S_b \Sigma_e}{S_f t_{fb}^2}[\sum_{j \neq f} p_{bj} + t_{bf}(1-t_{fb})]}$$

It should be noted that the right hand term in the denominator of the quotient is independent of the fuel cross section and can therefore be evaluated numerically.

Setting

$$X = \frac{S_b}{S_f t_{fb}^2}[\sum_{j \neq f} p_{bj} + t_{bf}(1-t_{fb})]$$

We can write the expression for the system fuel self collision probability as:

$$P = p_{ff} + \frac{\Sigma_t^f (1-p_{ff})^2}{\Sigma_t^f (1-p_{ff}) + X\Sigma_e}$$

We now introduce the Dancoff factor (γ) as the reduction in the fuel escape probability for an array of pincells relative to the fuel escape probability for an isolated pincell: the evaluation being carried out in the limit of black fuel.

$$\gamma = \frac{\lim it}{\Sigma_f \to \infty}(\frac{1-P}{1-p_{ff}})$$

The first flight fuel blackness (γ_f), that is, the probability that a neutron (entering the fuel with a cosine distribution about the normal to the fuel surface) will collide inside the fuel, without approximation, tends to unity in the limit of black fuel [3]. This gives:

$$\gamma_f = \frac{\lim it}{\Sigma_t^f \to \infty}\{\frac{\Sigma_t^f}{\Sigma_e}(1-p_{ff})\} = 1$$

Rewriting the expression for the system fuel self collision probability as:

$$\frac{1-P}{1-p_{ff}} = 1 + \frac{\frac{\Sigma_t^f}{\Sigma_e}(1-p_{ff})}{\frac{\Sigma_t^f}{\Sigma_e}(1-p_{ff}) + X}$$

and utilising the expressions for γ and γ_f in the limit of black fuel we obtain:

$$\gamma = 1 + \frac{1}{1+X}$$

or

$$X = \frac{\gamma}{1-\gamma}$$

The rational approximation is now introduced for both the cell and system fuel self collision probabilities such that:

$$p_{ff} = \frac{\Sigma_t^f}{\Sigma_t^f + a\Sigma_e} \quad \text{and} \quad P = \frac{\Sigma_t^f}{\Sigma_t^f + \alpha\Sigma_e}$$

therefore:

$$\frac{\Sigma_t^f}{\Sigma_t^f + \alpha\Sigma_e} = \frac{\Sigma_t^f}{\Sigma_t^f + a\Sigma_e} + \frac{\Sigma_t^f (1-p_{ff})^2}{\Sigma_t^f (1-p_{ff}) + \frac{\gamma}{1-\gamma}\Sigma_e}$$

After some algebra it can be shown that:

$$\alpha = \frac{a}{1 + \frac{a(1-\gamma)}{\gamma}}$$

The Dancoff factor is evaluated by numerical integration, using similar algorithms to the collision probability modules in WIMS, for an infinite array of pin cells arranged on either a square or triangular lattice (for PWR and VVER type lattices). The Dancoff factors for these regular lattices may be adjusted to give a first order correction for irregularities in the lattice, for example water gaps between assemblies or water filled guide tubes.

WIMS9 can also calculate Dancoff factors for cluster geometies and plate bundles. For these geometries effective values of Σ_p are determined for both a finite and an infinite lattice. For cluster geometries, the resonance shielding is greater in the centre of the cluster than on the outside where the pins are only shielded on one side. An approximate correction for this spatial effect is introduced by using infinite lattice values of Σ_p for all pins except the outer ring of pins. The resonance integral for the outer ring of pins (I_O) is then set such as to preserve the resonance integral of the average cluster pin I_C.

$$I_O = I_I + (I_C - I_I)\frac{M}{M_O}$$

Where I_I is the infinite lattice resonance integral, M is the number of pins in the cluster and M_O is the number of pins in the outer ring.

4.3 Summary of Equivalence Theory

The important points to note for equivalence theory are:

- A complex problem is related to homogeneous resonance integrals tabulated on the library.
- The value of the background scatter cross section σ_p, is adjusted to take account of the problem geometry, the other resonance nuclides in the problem and the type of moderator.
- The method is only applicable for simple geometries for which rational approximations to the fuel self collision probability can be determined.
- The fuel pellet is treated as a single region and therefore even if the fuel region is subdivided into a number of sub-regions by the user the same microscopic cross sections will be assigned to each sub region.
- Resonance overlap is calculated by a fine group slowing down calculation at lower energies.
- Corrections are made to the outscatter cross section, either based on a calculation of resonance escape probability or the fine group calculation.
- Current weighting is used to generate transport cross sections.

5 Sub-Group Theory

5.1 Introduction

The equivalence method in WIMS uses the concepts of Bell and Dancoff factors to derive an effective sigma-p value. This value is used as a look-up parameter in the WIMS library tables of resonance integral for each library energy group. The method is limited by the available algorithms for determining the so-called 'equivalent' sigma-p value in complex geometries; only for homogeneous systems, regular pin cell and plate arrays, and cylindrical clusters have the algorithms been coded in WIMS. Even for these, simplifying assumptions are made: in pins, only the volume average pin is available; in clusters, only two regions - inner and outer pins - are considered.

The sub-group method in WIMS was developed in order to be able to extend the resonance treatment to more complex geometries, originally the double heterogeneity of the Dragon HTR fuel elements, but more recently, a wide range of complex systems, including subdivisions of fuel pins.

As in the equivalence treatment, the sub-group method must yield broad group effective cross-sections that can be used in a standard coarse group, coarse mesh transport solution. Ideally, therefore, effective absorption, transport, scattering and fission cross-sections are required for all nuclides that are affected by resonance shielding. Also these cross-sections must be derivable from the data contained in the WIMS library, and in particular, from the existing tabulations of resonance integrals, which contain data as a function of library broad group, temperature and sigma-p.

5.2 Single Resonant Nuclides

In the description given in this section interactions between resonances of different resonant nuclides are not considered. A method of treating these interactions is discussed in the next section.

The definition of the broad group average resonance absorption cross-sections is:

$$\overline{\sigma}_a = \frac{\int \sigma_a(u)\phi(u,r)\,dr\,du}{\int \phi(u,r)\,dr\,du}$$

where $\phi(u,r)$ is the flux as a function of lethargy and position. This flux is itself a function of $\sigma_a(u)$, and hence the integrals contain only a single fundamental parameter that varies rapidly with lethargy. All other parameters that may be required to carry out this integration vary only slowly with lethargy, and this leads to an enormous simplification in the application of the method to the resonance energy range in WIMS. In the derivation, therefore, we shall assume that all parameters other than $\sigma_a(u)$ for

the resonance isotope being considered do not vary with lethargy, and that the library group averaged values can be used.

Even in a homogeneous case, this still leaves the two integrals in the numerator and denominator of the above equation to be evaluated. These integrals are of the form:

$$\int f(\sigma_a(u))du$$

The integrals may be cast in the form of summations, for example:

$$\int f(\sigma_a(u))du = \frac{\text{Limit}}{n \to \infty} \sum_{i=1}^{n} f(\sigma_a)_i \, w_i$$

Here, i denotes what is termed a sub-group and n the number of sub-groups. In a numerical calculation, a finite value of n is used, and it is sufficient to find the n values of σ_{ai} (the sub-group absorption cross-sections) and their corresponding sub-group weights w_i.

In order to minimise the number of sub-group calculations, the same set of subgroup cross-sections are employed for each library group. To implement this average values of resonance integrals are derived for the whole resonance region using a 1/E condensation spectrum. The library group dependence of the problem is then (almost) entirely represented by different sets of weights.

There is some evidence that this fitting procedure, adopted in WIMS, makes a small error of one sign in the high energy groups where there is little resonance shielding, and a small error of the opposite sign in the low energy groups where resonance shielding is most important. This is not surprising when a single set of sub-group cross-sections, optimised for an ‘average’ group, is used to cover the entire energy range.

To derive the sub-group cross-sections and weights requires no knowledge of the geometry and, arguably, it would be more efficient to store sub-group cross-sections as a function of temperature on the WIMS library. This would save time spent in the PRES module, but the saving would be small in the standard treatment. However, sub-group cross-sections could, in addition, be stored as a function of library group.

The derivation of the flux is identical to that used in homogeneous equivalence theory with the exception that the wide resonance approximation, rather than the intermediate resonance approximation is applied to the resonance scatter. The slowing down equation is therefore:

$$\left(\Sigma_a + \frac{\Sigma_{rs}}{\lambda} + \Sigma_{pot}\right)\phi = \frac{\lambda\Sigma_{pot}}{\bar{\xi}} + \left(\frac{\Sigma_{rs}}{\lambda} + (1-\lambda)\Sigma_{pot}\right)\phi$$

This lead to a flux of the form:

$$\phi(u) = \frac{\sigma_p}{\bar{\xi}(\sigma_p + \sigma_a(u))}$$

The expression for the broad group average resonance absorption cross-section becomes:

$$\bar{\sigma}_a = \frac{\int \frac{\sigma_a(u)\sigma_p}{\sigma_p + \sigma_a(u)} du}{\int \frac{\sigma_p}{\sigma_p + \sigma_a(u)} du}$$

The integrals are expanded in terms of a set of sub-group cross-sections and weights in the form:

$$\frac{\int \frac{\sigma_a(u)\sigma_p}{\sigma_p+\sigma_a(u)}du}{\int \frac{\sigma_p}{\sigma_p+\sigma_a(u)}du} = \frac{\sum_{i=1}^{n} \frac{w_i\sigma_a(\bar{u}_i)\sigma_p}{\sigma_p+\sigma_a(\bar{u}_i)}}{\sum_{i=1}^{n} \frac{w_i\sigma_p}{\sigma_p+\sigma_a(\bar{u}_i)}}$$

The resonance integrals of the data library are expanded in a similar form to give:

$$I_a\delta u = \int \frac{\sigma_a(u)\sigma_p}{\sigma_p+\sigma_a(u)}du = \sum_{i=1}^{n} \frac{w_i\sigma_a(\bar{u}_i)\sigma_p}{\sigma_p+\sigma_a(\bar{u}_i)}$$

As the resonance integrals are known these can be used to derive the cross-sections and weights as long as the number of sub-groups is less than or equal to half the number of tabulated values of the resonance integrals.

To obtain the correct form for the sub-group flux solution it is important to recognise there is a sub-group with zero absorption cross-section. This sub-group does not contribute to the fitting of the resonance integrals, the sub-group cross-section being zero, but does contribute to the flux. The weight associated with this sub-group is such as to make the sum of the sub-group weights add to unity. The flux is therefore given by:

$$\phi = \int \frac{\sigma_p}{\sigma_p+\sigma_a(u)}du = w_0 + \sum_{i=1}^{n} \frac{w_i\sigma_p}{\sigma_p+\sigma_a(\bar{u}_i)} \quad \text{where} \quad 1 = w_0 + \sum_{i=1}^{n} w_i$$

Therefore:

$$\phi = 1 - \sum_{i=1}^{n} w_i\left[1 - \frac{\sigma_p}{\sigma_p+\sigma_a(\bar{u}_i)}\right]$$

Giving:

$$\phi = 1 - \frac{1}{\sigma_p}\sum_{i=1}^{n} \frac{w_i\sigma_p\sigma_a(\bar{u}_i)}{\sigma_p+\sigma_a(\bar{u}_i)} = 1 - \frac{I_a}{\sigma_p}$$

Which can be seen to be of the correct form from Section 3.2 when there is only a single resonance nuclide present.

Having obtained these sub-group absorption cross-sections and weights the sub-group cross-sections for other reactions can be found by fitting their respective resonance integrals in the form:

$$\delta u I_x^s = \sum_{i=1}^{n} \frac{w_i\sigma_x^i}{1+\frac{\sigma_{a\,i}}{\sigma_{p,s}}}$$

Fission, scatter and removal are all considered as resonance reactions with resonance integrals held on the nuclear data library.

In practice, to reduce the number of flux solutions required, sub-group weights and absorption cross-sections are solved for the average resonance integrals across the resonance range rather than for each broad group separately. The condensation is performed over resonance groups g using:

$$I_x^s = \frac{\sum_g \delta u_g I_x^{s,g}}{\sum_g \delta u_g}$$

The absorption sub-group cross-sections and hence the total cross-sections are derived by the PRES module and output to a WIMS interface for use in a collision probability calculation. These sub-group cross-sections and collision probabilities are then used to derive sub-group fluxes for each sub-group i and in each region k of the j regions such that:

$$V_k \phi_k^i = \sum_j V_j P_{j,k}^i [\Sigma_{s,j}^i (1-\overline{\lambda})\phi_j^i + \overline{\lambda}\Sigma_{pot,j}]$$

Where P^I_{jk} is the first flight collision probability from region j to region k divided by the total sub-group cross-section for region k sub-group i. These collision probabilities are calculated from the total sub-group cross-sections defined, in terms of nuclides n, as:

$$\Sigma_{t,j}^i = \sum_n N_n^j [\sigma_{a,n}^i + \sigma_{pot,n}]$$

As an alternative to deriving subgroup collision probabilities, the CACTUS Characteristics module can be used to generate the subgroup fluxes directly. CACTUS carries out a fixed source calculation with the source set equal to the slowing down source above.

As pointed out before in this approximation the sub-group cross-sections, and hence sub-group fluxes, are broad group independent, the resonance integrals from which they are derived being the average resonance integrals over the resonance region. Broad group dependent weights are now defined for each sub-group i by fitting the broad group dependent resonance integrals for broad group g, nuclide n such that:

$$\delta u_g I_{a,g}^{s,n} = \sum_i \frac{w_i^g \sigma_{ai} \sigma_{p,s}}{\sigma_{ai} + \sigma_{p,s}}$$

In turn these broad group dependent weights are used to solve for the broad group dependent sub-group cross-sections for fission, scatter and removal. In general for reaction x:

$$\delta u_g (I_{x,g}^{s,n}) = \sum_i \frac{w_i^g \sigma_{x,g}^{n,i}}{1 + \frac{\sigma_a}{\sigma_{p,s}}}$$

The broad group average cross-sections can then be calculated by summing over the regions k containing the resonant nuclide:

$$\overline{\sigma}_{x,g}^n = \frac{\sum_k V_k \sum_i w_i^g \sigma_{x,g}^{n,i} \phi_k^i}{\sum_k V_k \sum_i w_i^g \phi_k^i}$$

In this way cross-sections are derived for resonance scatter, fission and removal. The group dependent fitting of sub-group cross-sections and the derivation of the broad group average cross-sections is performed by the WIMS RES module. RES also calculates the sub-group fluxes from the sub-group collision probabilities unless the option to input fluxes from CACTUS is used.

5.3 Interacting Resonance Nuclides

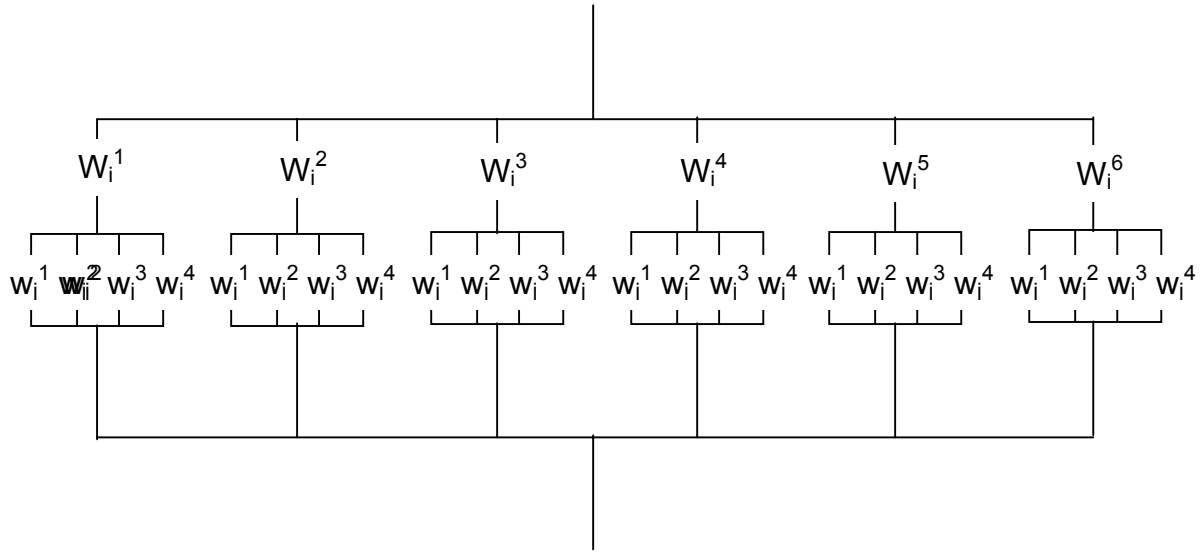
In the previous section the problem was treated as if there were only one resonance nuclide. To allow for interactions between the resonances of different resonance nuclides, WIMS uses a random statistical overlap model for the higher energy region of the resonance range, in which all combinations of sub-group interactions are allowed. For example, if there are two resonant nuclides with sub-groups denoted i and j respectively then all sub-groups i are subdivided by a further j sub-groups. Diagrammatically, assuming values of 6 and 4 for i and j respectively, this can be represented as in Figure 1.

Every combination of one nuclide's sub-group cross-sections are used with every combination of the other nuclide's sub-group cross-sections. The result is 24 sub-groups in total for each of which a flux must be calculated. The final broad group average cross-section for the nuclide with i sub-groups is given by:

$$\overline{\sigma}^{n}_{x,g} = \frac{\sum_k V_k \sum_i w_i^g \sigma^{n,i}_{x,g} \sum_j w_j^g \phi_k^{i,j}}{\sum_k V_k \sum_i w_i^g \sum_j w_j^g \phi_k^{i,j}}$$

If there were three nuclides interacting in the problem then every possible combination between the sub-groups of the three nuclides is considered. Usually, only two or at most three nuclides are treated as interacting as the number of flux calculations and computing time increases rapidly with the number of interacting nuclides.

Figure 1



In WIMS 9 this random overlap of resonances is assumed if the RANDOM keyword is given in the input data for RES. If this keyword is not given the resonance interaction factors calculated from the fine group calculation in HEAD are used with the uninteracted cross-sections from RES. Derivation of the uninteracted cross-sections in RES is discussed in Section 5.5.2.

5.4 The f(p) Correction

In WIMS 9 resonance integrals are available for both the resonance scatter and removal reactions, as well as absorption and fission, which, from the above theory yield broad group scatter and removal cross-sections. These cross-sections between them define the f(p) correction to be applied to the scattering matrix of the resonant nuclides. The scattering matrix is input to RES from the output created by the HEAD module. RES must normalise this matrix for each resonance nuclide, with components X(g->g'), such that:

$$\sum_{g'} \chi(g \rightarrow g') = 1.0$$

For resonant nuclides, denoted by n, the fraction of removal is defined by the derived scatter and removal cross-sections and a new scatter matrix must be constructed such that:

$$\frac{\overline{\sigma}_r^n}{\overline{\sigma}_s^n} = \sum_{g' \neq g} \chi'(g \rightarrow g')$$

The fraction of self, within group, scatter in the new matrix is therefore:

$$\frac{(\overline{\sigma}_s^n - \overline{\sigma}_r^n)}{\overline{\sigma}_s^n} = \chi'(g \rightarrow g)$$

Two multiplying factors are sought to convert the input scatter matrix from HEAD to produce the required output form from RES, one for the self scatter term and one for all other terms in the scatter matrix. The f(p) factor is defined as the multiplying factor for all terms in the input scatter matrix other than the self scatter, required to form the output scatter matrix. The f(p) factor is therefore:

$$\frac{\text{new\_removal\_fraction}}{\text{old\_removal\_fraction}} = f(p) = \frac{\overline{\sigma}_r^n}{\overline{\sigma}_s^n[1 - \chi(g \rightarrow g)]}$$

The output scatter matrix must still sum to unity and therefore the self scatter term is given by:

$$\text{self\_scatter\_fraction} = 1 - \frac{\overline{\sigma}_r^n}{\overline{\sigma}_s^n}$$

In terms of a multiplying factor, say g(p), to the input self scatter matrix term:

$$g(p) = \frac{(\overline{\sigma}_s^n - \overline{\sigma}_r^n)}{\overline{\sigma}_s^n \chi(g \rightarrow g)}$$

The above correction to the nuclide dependent scatter matrix is applied to the input scatter matrix by RES for the resonant nuclides only; this is valid whether or not the HEAD module has previously already applied an f(p) correction. RES makes no f(p) correction for the non-resonant nuclides as this is assumed to alredy have been applied by the HEAD module.

To maintain consistency between the P1 scatter matrix and the P0 scatter matrix both the P1 total scatter term and the P1 scatter matrix are scaled in the same way as the P0 terms. There is no directly available resonance shielded P1 scatter cross-section, however, if it is assumed the scaling is as for the P0 scatter then a scaling for the P1 scatter can be defined as:

$$\overline{\sigma}_{s1}^n = \frac{\overline{\sigma}_s^n}{\overline{\sigma}_s^n(\text{input})} \overline{\sigma}_{s1}^n(\text{input})$$

Here, input denotes the values read by RES from the interface, those output by HEAD. The scaling of the P1 scatter matrix is the same as for the P0 scatter matrix. Following the normalisation:

$$\sum_{g'} \chi_{s1}(g \rightarrow g') = 1.0$$

Then:

$$\chi'_{s1}(g \rightarrow g) = g(p)\chi_{s1}(g \rightarrow g)$$

For g not equal to g':

$$\chi'_{s1}(g \rightarrow g') = f(p)\chi_{s1}(g \rightarrow g')$$

In WIMS 8 there is no resonance scatter or removal cross-sections and none of these corrections to total scatter or the scatter matrix are applied.

5.5 Application of Fine Group Correction Factors

5.5.1 General

In WIMS the HEAD module calculates three types of correction factor which must be applied by RES these are:

- The resonance interaction correction, defined as:
  (Interacted cross-section)/(un-interacted cross-section)
- The absorption transport correction, defined as:
  (current weighted absorption cross-section)/(flux weighted absorption cross-section)
- The scatter transport correction, defined as:
  (current weighted scatter cross-section)/(flux weighted scatter cross-section)

These correction factors are only calculated by HEAD for broad groups 70 to 92 of the standard WIMS 172 broad group scheme. The fine group calculation from which they are derived is only valid at resonance energies where the 100 fine groups used within each broad group can give an adequate representation of the functional form of the resonance energy dependency. The application of these factors to this set of broad groups is described in the two sections below. WIMS 8 makes none of these corrections.

5.5.2 Resonance Interaction Correction

The resonance interaction, from its definition, must be applied to the un-interacted form of the cross-sections. Where sub-group theory has been used with two or more nuclides in interaction it is not obvious that the un-interacted cross-sections are available. However, these un-interacted cross-sections can be derived using the sub-group fluxes available. Consider the example of the last section where two resonant nuclides were considered with sub-groups denoted i and j with assumed values of 6 and 4 for the respective total numbers of sub-groups for i and j. Of the 24 sub-group flux solution 6 will represent cases in which nuclide i is represented with its six different sub-group cross-sections but nuclide j is represented with a zero sub-group absorption and resonance scatter cross-section. These six sub-group flux solutions exactly match the six sub-group flux solutions that would be solved if nuclide i had been in isolation without interaction. Likewise there are four flux solutions in which the resonance absorption and scatter sub-group cross-sections of nuclide i are zero but in which nuclide j is represented by each of its sub-group cross-sections respectively. To derive the un-interacted cross-sections simply requires an appropriate weighting and summation over the sub-group flux solutions:

$$\overline{\sigma}^{n}_{x,g} = \frac{\sum_k V_k \sum_i w_i^g \sigma^{n,i}_{x,g} \phi_k^{i,j=0}}{\sum_k V_k \sum_i w_i^g \phi_k^{i,j=0}}$$

The superscript of j = 0 indicates that the sub-set of flux solutions used is those in which the sub-group cross-sections of all the other resonance nuclides in the problem are zero. If f_x^n(int) is the interaction correction for nuclide n reaction x from the HEAD module then the final interacted cross-section is given by:

$$\overline{\sigma}_{x,g}^{n} = f_x^n(\text{int}) \frac{\sum_k V_k \sum_i w_i^g \sigma_{x,g}^{n,i} \phi_k^{i,j=0}}{\sum_k V_k \sum_i w_i^g \phi_k^{i,j=0}}$$

Note that this correction is only performed for the library groups 70 to 92 where the interaction correction calculation is valid. For groups higher than group 70 the random overlap interacted cross-sections calculated by RES are used without additional correction.

5.6 Summary of Subgroup Theory

The important points to note for subgroup theory are:

- As for equivalence theory, a complex problem is related to homogeneous resonance integrals tabulated on the library.
- Subgroup cross sections and weights are derived which when used in the slowing down equations reproduce the homogeneous resonance integrals tabulated on the library.
- The method can be applied to any geometry which can be modelled by collision probability methods or CACTUS.
- Resonance scatter is not included in the slowing down calculation.
- The cross section variation due to spatial geometry and fuel burnup can be represented to any degree of detail required.
- Resonance overlap is calculated by random interaction or by a fine group slowing down calculation at lower energies.
- Corrections are made to the outscatter cross section, based on factors calculated in the HEAD module.

6 References

1. S Glasstone and M C Edlund. The Elements of Nuclear Reactor Theory. D Van Nostrand Company Inc 1952.
2. Goldstein and Cohen. Nucl. Sci. Eng 13. 1962
3. R J Stamm'ler and M J Abbate. Methods of Reactor Physics in Nuclear Design. Academic Press 1983.

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