THE METHOD OF SUBGROUPS IN THE CALCULATION OF SHIELDED CROSS SECTIONS FOR WIMS–AECL

H. Chen and P.J. Laughton

Reactor and Radiation Physics Branch
AECL, Chalk River Laboratories
Chalk River, Ontario, Canada K0J 1J0 [613] 584–3311

ABSTRACT

The subgroups method provides a means of obtaining a spatial structure across a lattice cell of the neutron cross sections at resonance energies. This feature is absent in the equivalence principle that is currently employed by WIMS–AECL in obtaining shielded cross sections for heterogeneous cells. In addition, the calculation of the shielded cross sections by the method of subgroups is independent of the spatial geometry of a lattice cell, provided the collision probabilities are calculable. The method is therefore intended to be implemented in WIMS–AECL for the resonance treatment. A mechanism of implementing the method of subgroups into the calculation of shielded cross sections is presented. Preliminary results of the calculated shielded cross sections for ^{91}Zr in pressure tubes in a CANDU® lattice from the subgroups method and MCNP calculations are shown and discussed.

1 INTRODUCTION

There are two major goals of the subgroups method. The first is to achieve a more detailed spatial structure of the energy-group averaged, flux-weighted, cross sections, for isotopes such as ^{238}U and ^{239}Pu, when the neutron energies fall into the resonance range. These group-averaged cross sections are referred to as shielded cross sections. The name has its origin in the spatial self-shielding and energy self-shielding effects associated with the resonance phenomenon. Isotopes such as ^{238}U and ^{239}Pu are referred to as resonance absorbers because of the sharp resonances of their nuclear cross sections, which are found mainly in the epithermal range. The focus of the current work is on accounting for the self-shielding effect due to the resolved resonances in the epithermal region. A second objective is to obtain an enhanced flexibility in treating various fuel geometries.

A more detailed spatial structure of the shielded cross sections will lead to a more realistic spatial neutron-flux distribution, and a more accurate calculation of nuclear reaction rates, within a fuel bundle inside the core of a CANDU reactor. A geometry-independent formalism will allow the calculation of shielded cross sections for any fuel design to be carried out in a consistent way. The shielding of ^{91}Zr in the pressure tubes, for example, should receive no special treatment.

To illustrate the need for a detailed spatial structure of the shielded cross section, consider a pin cell where a cylindrical UO_2 (natural uranium) fuel pin is surrounded by D_2O moderator. Due to the large capture cross sections of ^{238}U at resonance energies, the mean-free-path of neutrons becomes rather small ($\approx$ 0.1 mm at 4000 barns). As a result, resonance neutron capture takes

CANDU® is a registered trademark of Atomic Energy of Canada Limited (AECL).

place mostly on the surface of a fuel pin, which leads to localized ^{239}Pu build-up and a rapid drop in neutron flux. This is known as the skin effect [1]. It also serves to demonstrate the effect of spatial self-shielding, as the ^{238}U nuclei inside the fuel pin are effectively shielded from capturing neutrons at resonance energies. The plutonium build-up affects the power distribution across a fuel pin, which in turn affects the temperature distribution across the fuel pin. A correct prediction of the power and temperature distributions requires an accurate calculation of the spatial variation of the neutron capture rate, which is determined by the shielded cross sections and the neutron flux. The subgroups method yields better estimates of the shielded cross sections at a finer spatial scale. This leads to the subsequent improvements of the calculated neutron flux distributions and the calculation of local nuclear reaction rates.

The shielded cross sections are defined by

$$\Sigma_{\mathrm{x},kg} = \frac{\sum_j n_k^j \int_{V_k} \int_{\Delta E_g} \sigma_{\mathrm{x},k}^j(E)\phi(\vec{r},E)\,dEdV}{\int_{V_k} \int_{\Delta E_g} \phi(\vec{r},E)\,dEdV} = \sum_j n_k^j \sigma_{\mathrm{x},kg}^j\,, \tag{1}$$

where $\Sigma_{\mathrm{x},kg}$ is the macroscopic shielded cross section for the spatial region k, energy group g and reaction x*. The corresponding microscopic shielded cross section for the isotope j is denoted by $\sigma_{\mathrm{x},kg}^j$. The number density for the isotope j at the spatial region k is represented by n_k^j, and it can always be chosen to be region-wise constant. The scalar neutron flux $\phi(\vec{r},E)$ is a function of the spatial variable $\vec{r}$ and energy E. The evaluation of the shielded cross sections is essentially determined by the evaluation of the flux-normalized resonance integrals, denoted by RI, where

$$\mathrm{RI} = \frac{\int_{V_k} \int_{\Delta E_g} \sigma_{\mathrm{x},k}^j(E)\phi(\vec{r},E)\,dEdV}{\int_{V_k} \int_{\Delta E_g} \phi(\vec{r},E)\,dEdV} \tag{2}$$

for isotope j and reaction x.

In WIMS–AECL, the neutron group flux ϕ_{kg}, averaged over some spatial region k and energy group g, is obtained by solving the multigroup neutron transport equation [2]:

$$\Sigma_{\mathrm{t},kg} V_k \phi_{kg} = \sum_{k'=1}^{K} V_{k'} P_{k'\to k,g} \left\{ \sum_{g'=1}^{G} \left(\sum_j \chi_g^j \left(\nu\Sigma_{\mathrm{f},k'g'}\right)^j + \Sigma_{\mathrm{s},k'g'\to g} \right) \phi_{k'g'} \right\}, \tag{3}$$

where $P_{k'\to k,g}$ is the collision probability corresponding to energy group g of width ΔE_g, from spatial region k' of volume $V_{k'}$ to spatial region k of volume V_k. The fission yield for group g and isotope j is denoted by χ_g^j, whereas G and K are the total number of energy groups and spatial regions, respectively.

To solve for the group flux ϕ_{kg} in the resonance region, the shielded cross sections such as $\Sigma_{\mathrm{t},kg}$, fission yields and collision probabilities for all k and g are first calculated. When the calculated results are taken as coefficients, Equation (3) becomes linear and can be easily solved for ϕ_{kg}. The only approximations inherent in Equation (3) are the isotropy of the emission density and the flat-flux-approximation (FFA) [3] with boundary conditions embedded in the collision probabilities. Clearly, if the solution of the group flux ϕ_{kg} is to be a good representation of the averaged neutron flux over the spatial region k and energy group g, the shielded cross sections, which themselves depend on the flux, must first reflect the true distribution of the neutron flux

*The symbol x can stand for fission, capture, elastic scattering and other nuclear reactions of interest.

in energy and space. Such characteristics of shielded cross sections are not easily obtained, due to the rapid change of cross sections of resonance absorbers with energy. Because of the rapid variation of the cross sections with energy, the neutron flux also changes rapidly with energy. In the case of a heterogeneous cell, the neutron flux also varies rapidly in space at the interface between absorbing and non-absorbing media, as the skin effect has demonstrated. Moreover, there are no known analytical solutions of the neutron flux when heterogeneity is present in a cell. The problem then becomes one of how to best describe the spatial and energy dependence of the shielded cross sections when the solution of the neutron flux is not known a priori.

2 THE CURRENT RESONANCE TREATMENT IN WIMS–AECL

Currently in WIMS–AECL, the calculations of shielded cross sections are based on the following principles:

In the case of a homogeneous cell [4, 5], the spatial variation of the flux is ignored. For an infinite homogeneous medium, it is possible to derive analytical solutions of the neutron flux as a function of energy under various approximations. Such solutions are taken as approximate weighting fluxes and are used to evaluate the RI. The weighting flux is usually parametrized by a dilution parameter σ_0, which is the total background scattering cross section per absorber atom. The resonance integral is then evaluated as a function of the dilution parameter for each absorbing isotope, and the results are stored in a nuclear data library.

When heterogeneity is present in a cell, as it is in all nuclear-power reactors, an equivalence principle is employed [6]. In cases where the cell geometry is simple, it can be shown [7] that if σ_0 is replaced by an *effective* background scattering cross section $\tilde{\sigma}_0$, the resonance integral for a heterogeneous cell is formally identical to that of the homogeneous case. Therefore, instead of evaluating the resonance integral for the heterogeneous cell directly, one needs only to compute the effective background scattering cross section $\tilde{\sigma}_0$ associated with the heterogeneous cell, and look up the corresponding value of the resonance integral previously stored for a particular absorber evaluated for a simple homogeneous cell.

There are two weaknesses associated with the equivalence principle when considering heterogeneous cells. First, the formalism derived from the equivalence principle depends on the fuel geometry in a cell. Therefore, one needs to derive a different equivalence relation with which to treat each different cell geometry, which makes the application of the equivalence principle inflexible. Furthermore, the effective background scattering cross section is derivable for simple geometries only. WIMS–AECL has, until recently, supported only a limited set of cell geometries. Secondly, the shielded cross sections calculated by WIMS–AECL have a rather coarse spatial structure. For example, in the case of a pin cell, the shielded cross section of a resonance group for the entire fuel region takes only one value. In other words, the shielded cross section so calculated is flat over the fuel region. Consequently, the spatial distribution of neutron flux calculated from these shielded cross sections has a limited spatial structure.

3 THE BASIC IDEA OF THE SUBGROUPS METHOD

The concept of subgroups was first introduced by Nikolaev almost thirty years ago in his study of the structure of resonance cross sections [8, 9]. Several applications based on his idea have been developed [5, 10, 11, 12, 13]. Our approach follows closely Nikolaev's original idea and has much in common with other implementations. Nevertheless, the means by which the subgroups

flux is calculated in this work is new.

The basic idea of the subgroups method is to divide neutrons that are in one particular broad energy group (in the resonance energy range) into smaller subgroups. The partition into subgroups is not carried out according to the energy of the neutrons; rather, the partition is made according to the total cross section at which the neutrons interact with a resonance absorber.

Figure 1 illustrates the subgroups concept. For a resonance absorber r in a resonance energy group g, the total cross section $\sigma_t^r(E)$ spans a range from $\sigma_{t,g}^{r,\min}$ to $\sigma_{t,g}^{r,\max\dagger}$. This range of total cross section is divided into I subsets, each of which is referred to as a subgroup. The I subgroups are bounded by a monotonically increasing sequence of points, $\sigma_{t,g}^{r,0}$, $\sigma_{t,g}^{r,1}$, ..., $\sigma_{t,g}^{r,i}$, ..., $\sigma_{t,g}^{r,I}$, where

$$\sigma_{t,g}^{r,i} < \sigma_{t,g}^{r,i'} \quad \text{if} \quad i < i' \tag{4}$$

and

$$\begin{aligned} \sigma_{t,g}^{r,0} &\leq \sigma_{t,g}^{r,\min} \\ \sigma_{t,g}^{r,I} &> \sigma_{t,g}^{r,\max} . \end{aligned} \tag{5}$$

Cross sections belonging to the range $\Delta\sigma_{t,gi}^r = \sigma_{t,g}^{r,i} - \sigma_{t,g}^{r,i-1}$ are said to be in the subgroup i. In the subgroups method, each subgroup i of cross sections is characterized by a single value, $\sigma_{t,gi}^r$, called the subgroup cross section for the subgroup i.

A subgroup i of neutrons within the energy group g, at some absorbing spatial region k, is defined to be the collection of neutrons of energies whose corresponding total cross sections belong to the subgroup i. This collection of neutrons constitutes the subgroup flux. When the set of cross sections corresponding to the subgroup i is characterized by the single subgroup cross section $\sigma_{t,gi}^r$, we define the subgroup flux (a density in energy), denoted by ϕ_{kgi}, to be the conventional neutron-flux density associated with this subgroup cross section $\sigma_{t,gi}^r$. Thus,

$$\phi_{kgi} \equiv \tilde{\phi}_k(\sigma_{t,gi}^r) . \tag{6}$$

Note that corresponding to each subgroup i of width $\Delta\sigma_{t,gi}^r$, there may be multiple subintervals ΔE_{gi}^m in energy where $m = 1, 2, ...$, as Figure 1 shows.

By introducing the concept of subgroups, the resonance integral can be replaced by a weighted sum of cross sections, thereby reducing the computational effort in evaluating the resonance integral associated with heterogeneous cells. At the same time, the method yields the desired spatial variation of the shielded cross sections. The evaluation of the resonance integral reduces to finding three quantities: the subgroup cross section, the subgroup flux and the subgroup weight, which is denoted by $\tilde{w}_{gi}$. As the following sections show, the subgroup weight is simply the sum of the energy intervals corresponding to the subgroup i within the broad energy group g.

---

†When referring to the boundary points of subgroups or subgroup quantities, namely the subgroup cross sections, the subgroup fluxes and the subgroup weights, the subscript g only denotes the energy group to which these quantities belong, and does not imply energy-group averaging.

4 THE SUBGROUP FLUX

It is assumed in this work that the neutron source density, denoted by $S_{k'}(E)$, averaged over some spatial region k', varies with energy E slowly enough within an energy group g of width ΔE_g such that it can be replaced by an energy-group averaged value, $S^a_{k'g}$. The neutron source density and its group-averaged value can take the following forms:

$$S_{k'}(E) = \int_0^\infty dE' \left\{ \sum_j \chi^j(E) \left(\nu\Sigma_{\mathrm{f},k'}(E')\right)^j + \Sigma_{\mathrm{s},k'}(E' \to E) \right\} \phi_{k'}(E') , \quad \text{and} \tag{7}$$

$$S^a_{k'g} = \frac{1}{\Delta E_g} \int_{\Delta E_g} S_{k'}(E) dE . \tag{8}$$

It can be shown [14], from the integral-transport equation for the scalar neutron flux, that this assumption leads to

$$\phi_k(E) = \tilde{\phi}_k \left(\Sigma_{\mathrm{t},k'}(E)\right) , \tag{9}$$

where $k' = 1, 2, ..., K$. If it is further assumed that the energy behaviour of $\Sigma_{\mathrm{t},k}(E)$ is dominated by that of a single resonance absorber, r, within the energy group g, Equation (9) simplifies to

$$\phi_k(E) = \tilde{\phi}_k \left(\sigma^r_{\mathrm{t}}(E)\right) . \tag{10}$$

Making use of the definition of the subgroup flux and ignoring the tildes for notational simplicity, we arrive at a means of calculating the subgroup flux ϕ_{kgi} given by

$$\Sigma_{\mathrm{t},kgi} V_k \phi_{kgi} = \sum_{k'=1}^{K} V_{k'} P_{k' \to k,i} S^a_{k'g} . \tag{11}$$

The macroscopic subgroup cross section $\Sigma_{\mathrm{t},kgi}$ in Equation (11) is related to its microscopic counterpart by

$$\Sigma_{\mathrm{t},kgi} = \sum_{j \neq r} n^j_k \sigma^{j,a}_{\mathrm{t},g} + n^r_k \sigma^r_{\mathrm{t},gi} \tag{12}$$

where the energy-group averaged microscopic cross section for each isotope $j \neq r$, within the energy group g, is denoted by $\sigma^{j,a}_{\mathrm{t},g}$. The cross sections $\sigma^{j,a}_{\mathrm{t},g}$ can be calculated, for various isotopes, using NJOY by assuming an approximate flux shape in each energy region. In the calculation of collision probabilities $P_{k' \to k,i}$, the macroscopic cross sections are taken to be energy-group averaged values for the non-absorbing spatial regions, and macroscopic subgroup cross sections for the absorbing spatial regions.

The discussion thus far in this section not only gives rise to a means of calculating the subgroup flux, it also reveals a situation that justifies the assumption at the heart of this neutron-subgroups method. Namely, in the resonance region, the energy behaviour of the neutron-flux density, averaged over some spatial region k, is dominated by that of the total cross section of some resonance absorber.

Equation (11) shows that the subgroup flux, ϕ_{kgi}, can be obtained through the collision probability calculations. Since the collision probability $P_{k' \to k,i}$ is dependent on the spatial region

of interest, k, the subgroup flux ϕ_{kgi} calculated from Equation (11) carries the signature of the spatial distribution of the neutron flux at energies at which the total cross section is $\Sigma_{t,kgi}$ for a given lattice cell. This introduces the desired spatial dependence into the shielded cross sections.

A set of computer programs called SFLUX was written to perform the subgroup flux calculations. The cross sections needed in calculating the source term $S^a_{k'g}$ are taken as unshielded.

5 THE LEBESGUE INTEGRATION SCHEME AND SHIELDED CROSS SECTIONS

The concept of subgroups simplifies the evaluation of the resonance integral by allowing it to be carried out in the Lebesgue integration scheme. A brief explanation of this scheme is given below.

Suppose we have some function, $f_k\left(\sigma_t^r(E)\right)$, that varies rapidly with E over a range of energy, ΔE_g. The function itself varies between $f_k^{\min}$ and $f_k^{\max}$. Evaluating the integral in the usual Riemann scheme, we have

$$\int_{\Delta E_g} f_k\left(\sigma_t^r(E)\right) dE = \lim_{n\to\infty} \sum_{i=1}^{n} f_{k,E} \Delta E_i \tag{13}$$

where $f_{k,E}$ is a representative value of $f_k\left(\sigma_t^r(E)\right)$ in the subinterval, ΔE_i. If the width of the peak is less than or comparable to ΔE_i, the numerical evaluation of the integral, which is always a finite sum, can be far from the true integral, unless special measures are employed, which usually are time-consuming.

In the Lebesgue integration scheme [15], a partition on the integrand between $f_k^{\min}$ and $f_k^{\max}$ is carried out, as shown in Figure 2. Evaluated in the Lebesgue sense, we have

$$\int_{\Delta E_g} f_k\left(\sigma_t^r(E)\right) dE = \lim_{n\to\infty} \sum_{i=1}^{n} f_{k,i} \mathcal{M}_i \tag{14}$$

where $f_{k,i}$ is a characteristic value of the function f_k within the interval Δf_i, and $\mathcal{M}_i$ is the corresponding Lebesgue measure for the interval Δf_i, and is simply the sum of the energy subintervals within which the corresponding values of the function f_k belong to the interval Δf_i. For large and narrow peaks, the Lebesgue integration scheme naturally divides the peaks into pieces and leads to a better representation of the true integral when using finite sums. The advantage of using the Lebesgue integration scheme when evaluating the resonance integral thus becomes intuitive.

Employing the approximation that the neutron flux is a function of the total microscopic cross section of a resonance absorber, the numerator of the resonance integral for absorber r and reaction x=t can be written as

$$\mathrm{RI}_t^{\mathrm{nu}} = \int_{\Delta E_g} \sigma_t^r(E) \phi_k\left(\sigma_t^r(E)\right) dE = \int_{\Delta E_g} f_k\left(\sigma_t^r(E)\right) dE \tag{15}$$

where $f_k\left(\sigma_t^r(E)\right) = \sigma_t^r(E)\phi_k\left(\sigma_t^r(E)\right)$ is a function of the total cross section. Recognizing that $f_k\left(\sigma_t^r(E)\right)$ is a single-valued function of $\sigma_t^r(E)$ within the energy group g, instead of partitioning strictly the integrand f_k, one can partition the cross section $\sigma_t^r(E)$, of which f_k is a function. For

each resulting subgroup cross section $\sigma^r_{t,gi}$, there corresponds a uniquely defined value in f_k, which we denote by f_{kgi} and

$$f_{kgi} = \sigma^r_{t,gi}\phi_{kgi} \tag{16}$$

where ϕ_{kgi} is calculated by Equation (11). Bear in mind that $\sigma^r_t(E)$ is a single-valued function of E. It is then seen that the sum of subintervals in energy corresponding to a subgroup $\Delta\sigma^r_{t,gi}$ is the Lebesgue measure of the subgroup i, which we denote by ΔE_{gi}.

Carried out in the Lebesgue sense, the integral of Equation (15) becomes an infinite sum of the elementary areas $f_{kgi}\Delta E_{gi}$. Thus,

$$\int_{\Delta E_g} f_k\left(\sigma^r_t(E)\right) dE = \lim_{I\to\infty}\sum_{i=1}^{I}\sigma^r_{t,gi}\phi_{kgi}\Delta E_{gi} = \lim_{I\to\infty}\sum_{i=1}^{I} f_{kgi}\Delta E_{gi}\,. \tag{17}$$

Conforming to the nomenclature of the subgroups method, ΔE_{gi} is also termed the subgroup weight denoted by $\tilde{w}_{gi}$. With the normalization constraint $\sum_i w_{gi} = 1$, the subgroup weight w_{gi} becomes

$$w_{gi} = \frac{\Delta E_{gi}}{\Delta E_g} = \frac{\sum_m \Delta E^m_{gi}}{\Delta E_g}\,. \tag{18}$$

Clearly, as long as the boundary points of the subgroups are known, the subgroup weights w_{gi} can be evaluated from the point-wise cross-section data.

The motive for partitioning $\sigma^r_t(E)$ between $\sigma^{r,\min}_{t,g}$ and $\sigma^{r,\max}_{t,g}$ for a given energy group g is two-fold. First, $\sigma^r_t(E)$ is a rapidly varying function of E within the resonance region. Based on the merits of the Lebesgue integration scheme, it is more efficient to partition $\sigma^r_t(E)$ than to partition E. Second, the shape of $\sigma^r_t(E)$ as a function of E is only a property of the isotope. Therefore, it is possible to derive, in advance, the subgroup cross sections and the subgroup weights without knowing the geometry of the lattice cell, and store the results. On the other hand, $f_k\left(\sigma^r_t(E)\right)$ must be calculated for every $\sigma^r_t(E)$ and for every specific geometry, which makes an a priori determination of the subgroup constants via f_k rather limited.

For details on a method to evaluate subgroup cross sections and subgroup weights, see the companion paper [16] published in these proceedings.

Once all three subgroup quantities (namely, the subgroup cross section, the subgroup flux and the subgroup weight) are calculated, the shielded cross sections take the form

$$\sigma^r_{x,kg} = \frac{\sum_{i=1}^{I}\sigma^r_{x,gi}\phi_{kgi}w_{gi}}{\sum_{i=1}^{I}\phi_{kgi}w_{gi}}\,, \tag{19}$$

which shows that they are simply weighted sums of cross sections. A computer program called SRXS was written to perform calculations of the shielded cross sections using the subgroups method.

The advantages of the subgroups method are summarized below:

- It gives rise to the spatial structure of the shielded cross sections that is absent in the equivalence principle-based models.
- The formalism is independent of the geometry of the lattice cell, which means that it can be applied to any fuel design provided the collision probabilities are calculable.

- The subgroup constants can be prepared in advance, once only, for all resonance isotopes with a predetermined number of subgroups.

6 PRELIMINARY RESULTS AND DISCUSSIONS

Self-shielding calculations were performed for the $g = 31$ energy group in the WIMS–AECL ENDF/B-based libraries, for ^{91}Zr in a CANDU-reactor pressure tube. This energy group is bounded by 275.36 eV and 454 eV. In this energy range, ^{91}Zr displays two resonances (see Figure 1 of Reference 16).

The problem geometry was of the simple annular type. The pressure tube was subdivided into ten cylindrical regions where the increment in radius between the adjacent cylindrical surfaces is 0.45 cm. To simplify the problem, it was assumed that the space inside and outside the pressure tube contains heavy water. The number of subgroups in this case was set to be $I = 4$. Calculations were carried out using SRXS and MCNP on the shielded total and shielded absorption cross sections. Results are shown in Figures 3 and 4.

The figures show the calculated shielded cross sections from the inner radius (5.17 cm) of the pressure tube to its outer radius (5.62 cm). The subgroups method gives the correct feature of the spatial variation of the shielded cross sections; its results and those from the MCNP calculations reveal the same trend. The unshielded cross sections are also displayed to illustrate the magitude of the self-shielding effect.

Discrepancies between the SRXS and the MCNP calculations are to be expected. Source of discrepancies built into SRXS include: the approximation of constant source density per unit energy; the discontinuous multigroup nature of SRXS; and the assumption of isotropic scattering, all of which are not assumed in the Monte Carlo (MCNP) calculations. In addition, the number of subgroups and the constraints placed in obtaining the subgroup parameters could have an impact on the calculated values of the shielded cross sections. The magnitude of the error introduced by these approximations is not easy to quantify without extensive investigations. A planned immediate investigation is to use a constant source density per unit lethargy instead of that per unit energy employed in the present work as indicated in Equation (8). It is known that the source density per unit lethargy in the slowing-down range, in the case of an infinite, non-absorbing, homogeneous medium with slowly-varying scattering cross sections, can be approximated well as constant over an energy group (such as the $g = 31$ group). Thus, a constant source density per unit lethargy is likely a less severe approximation than a constant source density per unit energy.

The ratio of shielded to unshielded cross sections serves as a measure of the impact on the neutron balance in a nuclear reactor from resonance self-shielding. Consider the ratio of the shielded microscopic cross sections derived from MCNP to the unshielded cross sections, and the same ratio evaluated with SRXS instead of MCNP. The volume-weighted average of the difference between these two ratios is about 0.07 for the absorption cross section and 0.13 for the total cross section. These results are considered to be good. Nevertheless, discrepancies between the MCNP calculations and the SRXS calculations exist and remain to be explained. It is known, however, that errors introduced by an underprediction of shielded cross sections are generally compensated by an overprediction of the neutron-flux densities and vice versa [7]. Thus, we expect superior agreement with MCNP calculations when the reaction rate, which is proportional to the product of the shielded cross section and the corresponding neutron-flux density, is to be evaluated. Also noteworthy is that because the effect on the overall neutron balance from neutron absorption is primary, while that from neutron scattering is secondary, the level of agreement of the calculated shielded absorption

cross sections is of greater importance than that of the shielded total cross sections.

The calculation of the shielded cross sections for ^{91}Zr is not available from WIMS–AECL for comparison, since WIMS–AECL currently only shields fuel materials, and the problem geometry used here cannot be handled directly by the self-shielding methods of WIMS–AECL as they now stand. Calculations of the shielded cross sections of ^{238}U are ongoing for comparisons between WIMS–AECL, SRXS and MCNP results.

ACKNOWLEDGEMENTS

The authors wish to acknowledge NSERC and COG Working Party 25 program 2501 for supporting this work.

REFERENCES

1. M. Wagner. Spatial distribution of resonance absorption in fuel elements. *Nuclear Science and Engineering*, 8:278–281, 1960.

2. D.W. Anderson. The WIMS–E module W–PIJ. A two-dimensional collision probability code with general boundary conditions. AEEW–R 862, United Kingdom Atomic Energy Authority (Atomic Energy Establishment, Winfrith), Dorchester, Dorset, England, 1973 September.

3. H. Chen. Unpublished internal report, AECL (Chalk River), 1996 April.

4. R.J.J. Stamm'ler and M.J. Abbate. *Methods of Steady-State Reactor Physics in Nuclear Design.* Academic Press, London, England, 1983.

5. M.J. Roth. Resonance absorption in complicated geometries. AEEW–R 921, United Kingdom Atomic Energy Authority (Atomic Energy Establishment, Winfrith), Dorchester, Dorset, England, 1974 March.

6. J.V. Donnelly. Description of the resonance treatment in WIMS–AECL. AECL Report, AECL–10550, 1993 May.

7. Allan F. Henry. *Nuclear Reactor Analysis.* M.I.T. Press, Cambridge, MA, 1975.

8. M.N. Nikolaev and V.V. Filippov. Measurements of the resonance structure parameters of the total cross sections of some elements in the neutron energy range 0.3 - 2.7 MeV. *Soviet Atomic Energy*, 15:493–498, 1963.

9. M.N. Nikolaev, A.A. Ignatov, N.V. Isaev and V.F. Eokhlov. The method of subgroups for considering the resonance structure of the cross sections in neutron calculations (part 1). *Soviet Atomic Energy*, 29:689–695, 1970.

10. D.E. Cullen. Application of the probability table method to multigroup calculations of neutron transport. *Nuclear Science and Engineering*, 55:387–400, 1974.

11. M.V. Gregory. A correlation technique for resonance calculations. *Nuclear Science and Engineering*, 71:59–64, 1979.

12. O.K. Bouhelal and P. Ribon. Reference tabulation of neutron data by the concept of probability tables. *Appl. Radiat. Isot.*, 46:551–552, 1995.

13. V.V. Tebin and M.S. Yudkevich. Generalized subgroup approach to calculating the resonant absorption of neutrons. *Soviet Atomic Energy*, 59:96–101, 1984.

14. H. Chen and P.J. Laughton. Unpublished internal report, AECL (Chalk River), 1997 July.

15. V.I. Ilyushchenko. New integration methods of global optimization based on Riemann, Lebesgue and Perron integral structures. In *Communication of the Joint Institute for Nuclear Research, Bubna*, number JINR E10-90-552, 1990.

16. P.J. Laughton. On the preparation of library data for an implementation of the method of subgroups in WIMS–AECL. In *Proceedings of the 1997 Nuclear Simulation Symposium*, Niagara-on-the-Lake, Ontario, 1997 September. Canadian Nuclear Society.

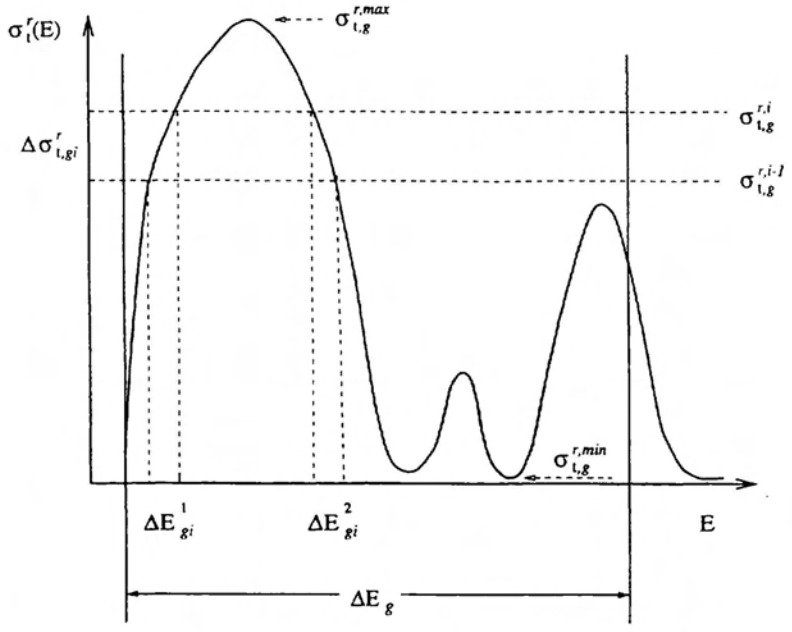

Figure 1: An illustration of a subgroup $\Delta\sigma_{t,gi}^r$ of cross sections and its corresponding subgroup weight $w_{gi} = \Delta E_{gi}^1 + \Delta E_{gi}^2$.

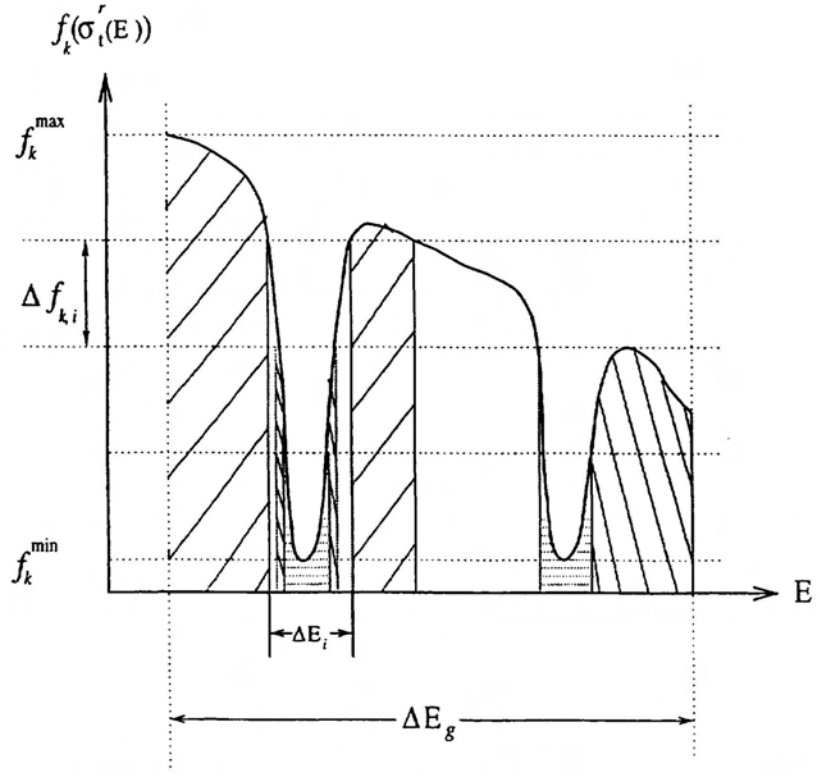

Figure 2: An illustration of the Riemann and Lebesgue integration schemes.

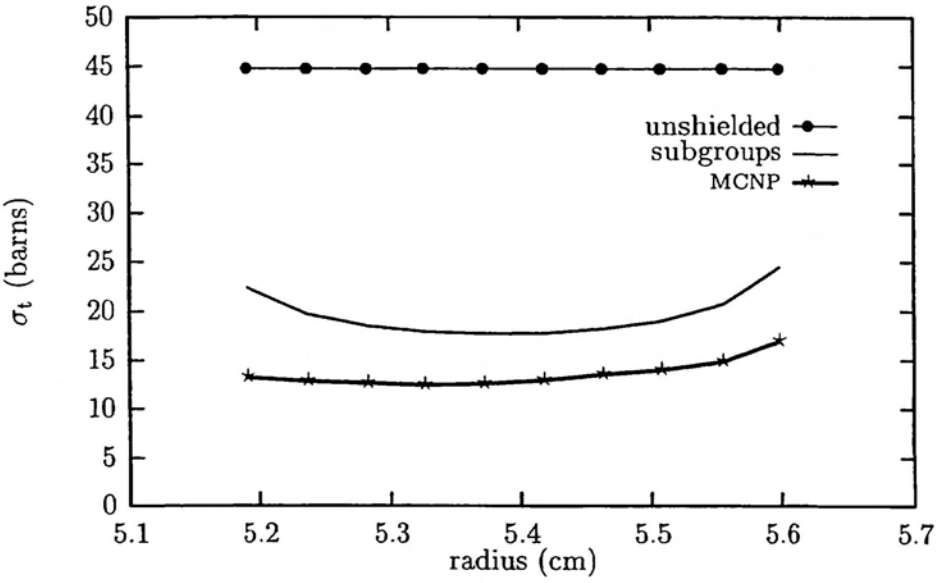

Figure 3: Shielded total cross sections of ^{91}Zr for energy group $g = 31$.

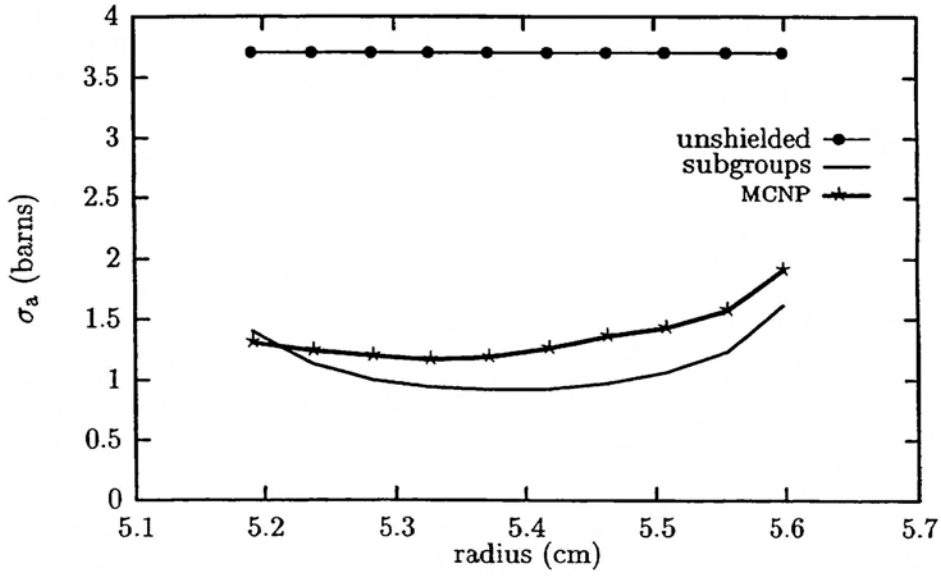

Figure 4: Shielded absorption cross sections of ^{91}Zr for energy group $g = 31$.