Homogenized Group Cross Sections by Monte Carlo

S.C. van der Marck, J.C. Kuijper, and J. Oppe
Nuclear Research and Consultancy Group NRG, Westerduinweg 3, Petten, the Netherlands

Abstract

Homogenized group cross sections play a large role in making reactor calculations efficient. Because of this significance, many codes exist that can calculate these cross sections based on certain assumptions. However, the application to the High Flux Reactor (HFR) in Petten, the Netherlands, the limitations of such codes imply that the core calculations would become less accurate when using homogenized group cross sections (HGCS). Therefore we developed a method to calculate HGCS based on a Monte Carlo program, for which we chose MCNP. The implementation involves an addition to MCNP, and a set of small executables to perform suitable averaging after the MCNP run(s) have completed. Here we briefly describe the details of the method, and we report on two tests we performed to show the accuracy of the method and its implementation. By now, this method is routinely used in preparation of the cycle to cycle core calculations for HFR.

KEYWORDS: homogenized group cross sections, Monte Carlo, macroscopic, microscopic

1. Introduction

Homogenized group cross sections play a large role in making reactor calculations efficient. Because of this significance, many codes exist that can calculate these cross sections based on certain assumptions. However, the application to the High Flux Reactor in Petten (the Netherlands), the limitations of such codes imply that the core calculations would become less accurate when using homogenized group cross sections (HGCS). This is because the experiments irradiated in this reactor, and the isotope production facilities in it, are heterogeneous in the extreme, and moreover sometimes contain isotopes with a large absorption cross section (such as ^{191}Ir). Also, they may contain water that acts as a flux trap, or uranium targets that add to the reactivity of the core. The reactivity effect of many of these experiments is of the order of 300–400 pcm (roughly half a dollar) per experiment.

Therefore we require a method to calculate HGCS using a Monte Carlo program, enabling us to cope with any situation, no matter how complicated it may be neutronically. A proof of principle was given in Ref. [1], where group cross sections were calculated using MCNP. Although a 'patch file' for MCNP is given in Ref. [1], it is for an older version (4A), and it involves an implementation that slows down MCNP by a factor 2~10. Also the Monte Carlo program VIM [2] can calculate group cross section, but this code it not used as widely as MCNP, which is the Monte Carlo program of choice for us.

We first tried to obtain all the necessary information by means of suitable tallies in MCNP. Since HGCS are defined by means of reaction rates, most of these tallies would need to be reaction rate tallies. Supposing we want HGCS for several processes, such as elastic scattering, inelastic scattering, absorption, fission, (n,2n), (n,3n) in, say, 10 zones containing e.g. 20 isotopes each, this would entail 1200 reaction rate tallies. In MCNP these reaction rate tallies are track length tallies, making this process very slow: for each part of a neutron track all these reaction rates would need to be evaluated for all isotopes in the zone, irrespective of whether such a reaction was actually simulated. The resulting run times become prohibitive. It is for this same reason that the implementation in Ref. [1] is slow.

The logical next step is to use collision estimators for these tallies, but these are unavailable in MCNP. Therefore we created another feature in MCNP. We programmed the possibility to have MCNP print a record in a binary file for each interaction that is simulated. On this record all the necessary data for later post-processing are present, like position, reaction type, energies, angle. The number of records in the file for a particular reaction in a volume is proportional to the reaction rate in that volume. Suitable post-processing can rework the information, and, in combination with just a few standard MCNP tallies, produce HGCS for all reaction types that MCNP simulates. Obviously the use of a large binary file, typically Gb size, is a drawback. It is not problematic, though, because it is only a temporary file.

We have written a tool, ELNINJO (for Elementary Nuclide Inventory Journal), to perform the post-processing tasks. The tools needs as input the binary file containing collision data, one flux tally (f4) containing MCNP results for all the zones for which HGCS are to be calculated, and one reaction rate tally (f4+fm4) for normalization purposes. We have tested the produced HGCS in several ways. In this paper we report on the methods that are encoded in ELNINJO (next section) and on two tests we have performed (the section thereafter). The geometries employed in these tests are related to the actual situation in the High Flux Reactor in Petten, the Netherlands [3]. The first test model consists of half a fuel plate assembly and half a water reflector, with reflective boundary conditions. For the second test we considered two specific experiment types and calculated their influence on reactor core calculations using detailed models and using HGCS.

2. Theory

Homogenized group cross sections are defined as the cross section that preserves reaction rates. For a reaction x of nuclide i in energy group g in volume V the reaction rate is given by

$$R^{(i)}_{xg} = \int d^3\mathbf{r} \int dE \ \sigma^{(i)}_x(E,\mathbf{r}) \ \varphi(E,\mathbf{r}) \ N^{(i)}(\mathbf{r}) \quad (1)$$

$$\equiv \underline{\underline{\sigma}}^{(i)}_{xg} \ \underline{\varphi}_g \ \underline{\underline{N}}^{(i)} \ V. \quad (2)$$

Here σ denotes the cross section, φ the (local) flux, and N the (local) nuclide density. We use the notation $\underline{\underline{\sigma}}$ for the homogenized microscopic group cross section, $\underline{\varphi}$ for the averaged group flux, and $\underline{\underline{N}}$ for the averaged nuclide density. The latter is defined as

$$\underline{\underline{N}}^{(i)} \equiv 1/V \int d^3\mathbf{r} \, N^{(i)}(\mathbf{r}), \quad (3)$$

while the average flux is defined by

$$\underline{\varphi}_g \equiv 1/V \int d^3\mathbf{r} \int dE \ \varphi(E,\mathbf{r}). \quad (4)$$

The homogenized macroscopic cross section can then be calculated as

$$\underline{\underline{\Sigma}}^{(i)}_{xg} = R^{(i)}_{xg}/(\underline{\varphi}_g V), \quad (5)$$

and the homogenized microscopic one as

$$\underline{\underline{\sigma}}^{(i)}_{xg} = R^{(i)}_{xg}/(\underline{\varphi}_g \underline{\underline{N}}^{(i)} V). \quad (6)$$

For reactions with outgoing neutrons one needs an outgoing neutron energy group g' as well, so that in this case the homogenized macroscopic cross section reads $\underline{\underline{\Sigma}}^{(i)}_{xgg'} = R^{(i)}_{xgg'}/(\underline{\varphi}_g V)$, and $\underline{\underline{\sigma}}^{(i)}_{xgg'} = R^{(i)}_{xgg'}/(\underline{\varphi}_g \underline{\underline{N}}^{(i)} V)$ for the microscopic one. Information on the angular distribution of outgoing neutrons is contained In the so-called "cosine rate" $M^{(i)}_{xgg'}$

$$M^{(i)}_{xgg'} = \int d^3\mathbf{r} \int dE \int dE' \ \mu^{(i)}_x(E,E') \ \sigma^{(i)}_x(E,E',\mathbf{r}) \ \varphi(E,\mathbf{r}) \ N^{(i)}(\mathbf{r}) \quad (7)$$

$$\equiv \underline{\mu}^{(i)}_{xgg'} R^{(i)}_{xgg'}. \quad (8)$$

$\mu^{(i)}_{xgg'}$ is the average cosine between the incoming neutron (in energy group g) and the outgoing neutron (in energy group g') for reaction x.

This can be suitably summed over the outgoing energy groups g' and over the elastic and inelastic scattering reactions x, the result of which we denote by $M^{(i)}_{Sg}$. The transport corrected total cross section, or the 'transport cross section', is calculated by ELNINJO in both the outscatter and the inscatter approximation (see e.g. the SCALE manual [4]). For the macroscopic tranport cross section in the outscatter approximation the equation

$$\underline{\underline{\Sigma}}^{(i)}_{tr,g} = \underline{\underline{\Sigma}}^{(i)}_{T,g} - M^{(i)}_{S,g}/(\underline{\varphi}V) \quad (9)$$

is used, with Σ_T the total cross section. For the inscatter approximation of the transport cross section we define $N^{(i)}_{Sg}$ as the sum over g' of $M^{(i)}_{Sg'g}$ (note that this sum is over the incoming energy groups), so that

$$\underline{\underline{\Sigma}}^{(i)}_{tr,g} = \underline{\underline{\Sigma}}^{(i)}_{T,g} - N^{(i)}_{S,g}/(\underline{\varphi}V). \quad (10)$$

It should be noted that for the inscatter approximation ELNINJO uses the flux φ instead of the neutron current, assuming that the flux spectrum is a good approximation for the current spectrum.

The microscopic cross sections can be obtained from the macroscopic ones by dividing by the average nuclide densities in the zone. In general, these average densities are not known, since the zones for which we calculate HGCS do not need to coincide with MCNP cells. This problem can be overcome by performing a void run with a tally definition that lets MCNP calculate the volume per zone per cell. Using this as extra input, ELNINJO works out the average nuclide densities in each zone.

3. Tests

Our first test consisted of half a fuel plate assembly with adjacent water, see Fig. 1. Reflecting boundary conditions were used in all directions. We calculated HGCS in seven energy groups for this system in two zones: the left half, containing fuel plates, cladding, and water, and the right half, containing only water. These HGCS were fed into PANTHER [5], in which the flux distribution was re-calculated on a 40×20 sub-mesh. This flux profile compares well with flux results from the original MCNP runs. One can also compare values for k_∞ for this system, see Table 1. The results based on HGCS are close to the k_∞ values from the original MCNP runs. We also performed the same test on HGCS produced by WIMS [6], for which the k_∞ results were also close to the original WIMS results, but not as close as for ELNINJO.

Figure 1. The one-dimenional geometry of the model for the first test of ELNINJO (see test).

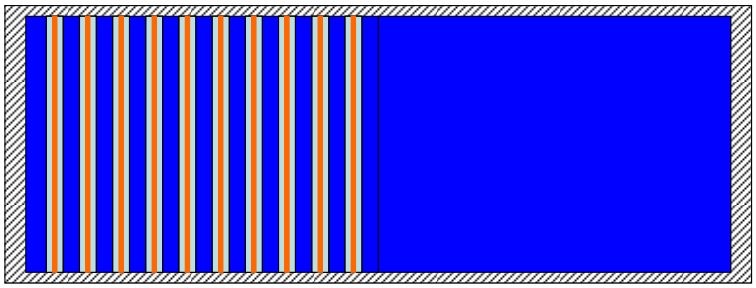


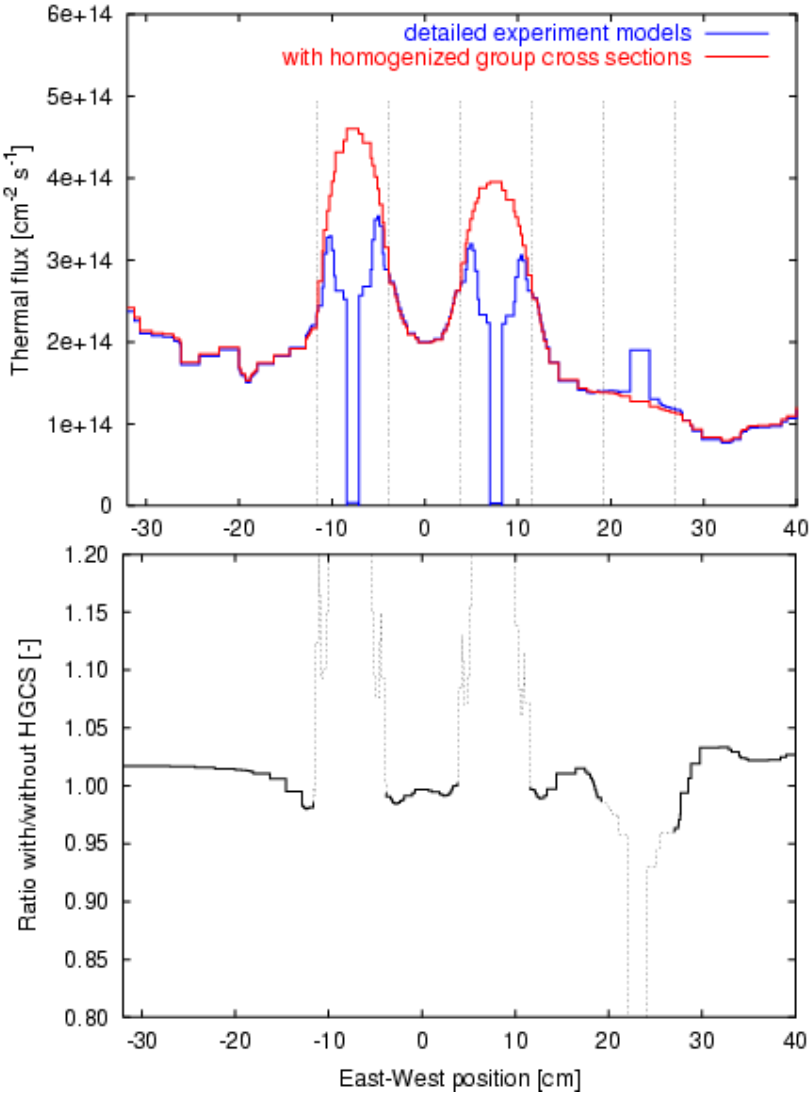
Table 1. Results obtained using homogenized group cross sections from ELNINJO, compared with original MCNP model, and compared with another method of calculating group cross sections.

	k_∞	$\delta\rho$
MCNP	1.32672 ± 0.00010	
ELNINJO → PANTHER, inscatter	1.32992	181 pcm
ELNINJO → PANTHER, outscatter	1.32431	–137 pcm
WIMS	1.33787	
WIMS → Panther	1.33024	–428 pcm

Our second test was to use HGCS for all 17 experimental positions in core calculations for the High

Flux Reactor at Petten (the Netherlands). We used REBUS [7] to calculate the power and flux distributions for the reactor core in two ways: once based on detailed Rebus model of these experiments, and once based on HGCS from ELNINJO (and converted into an ISOTXS library). An example of the results is given in Fig. 1, where the thermal flux along a central line through the reactor is shown.

Figure 2. The thermal flux results for the High Flux Reactor, using detailed experiment models (blue) and using homogenized group cross sections (red) in REBUS. In the Figure below, the ratio between the two curves is plotted.

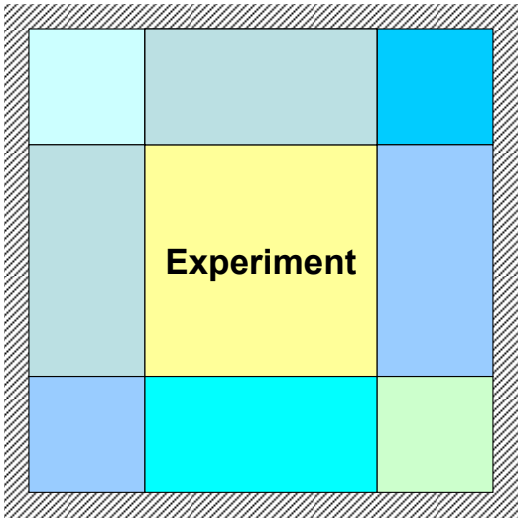


It can be seen that the fluxes within the experimental positions differ between the two calculational methods. This is allowed, since the HGCS are based on conservation of reaction rates, not flux. In fact, in the detailed experiment model at positions −8cm and at +8cm in Figure 1, an internal black boundary condition was used in Rebus, whereas this boundary condition is absent when using HGCS. The real test is whether the description of flux and power outside the experimental positions is correct. The figure shows that this indeed the case: the ratio between the two methods is easily within 5% from unity outside the experiments.

Having performed these tests with good results, we are using this method on a routine basis for the core calculations for the HFR during the conversion to LEU [8]. For each experiment that is deemed to have a sizable influence on the core, an MCNP model is available. This model is then put inside a 3x3

environment with reflecting boundary conditions, see Fig. 2.

Figure 3. The environment in which homogenized group cross sections are calculated for the HFR cycle calculations.



One might argue that it is better to use an even more representative environment for the calculation of HGCS, but since the abovementioned second test gave good results, we have not explored this further. Each neighbouring position is represented by half its size (or a quarter on the edges) because of the boundary conditions. The material definition for each of the neighbours is taken to be an average over the whole position, based on historical (HEU) cycles. Once this model is complete, the rest of the calculation is automated. Using a few linux-scripts, the necessary two or three MCNP runs are performed, and after that the ELNINJO post-processing is started automatically. The last action in this chain is the conversion of the HGCS data to either ISOTXS (for use in REBUS) or HEADE format (for use in OSCAR-3 [9]). All runs and post-processing typically take roughly three to four hours elapse time on a set of standard out of the box PCs configured with linux.

4. Conclusions

We conclude that we have a tool to construct HGCS from Monte Carlo calculations. This tool is very general and can handle any geometric complexity as well as any amount of absorption, fission, or moderation. The zones for which the HGCS are calculated can be smaller than MCNP cells, can be larger, and can even cut through them. The calculated group cross sections can be expressed as microscopic ones or as macroscopic ones, both in 1D and in 2D. At this moment the results of the post-processing tool calculates diffusion theory parameters, which can be used in both diffusion theory codes and transport theory codes. The method can easily be extended to generate data for higher order moments of the scattering matrix. ELNINJO has been tested extensively, and has served us well in supporting the core calculations during the conversion to LEU of the High Flux Reactor.

1) E.L. Redmond, “Multigroup cross section generation via Monte Carlo methods”, PhD Thesis MIT, 1997
2) R.N. Blomquist, “VIM, 3-D Monte Carlo analysis of fast critical assemblies using point cross sections”, www.nea.fr/abs/html/nesc0510.html
3) www.nrg-nl.com/product/irradiat/hfr
4) N.M. Greene and L.M. Petrie, “XSDRNPM-S: a one-dimensional discrete-ordinates code for transport analysis”, ORNL (1983)

5) P.K. Hutt et al, "The UK Core Performance Package", Nucl. Energy **30** (1991) 291
6) "WIMD – a modular system for neutronics calculations – user guide for version 8", AEA Technology – Nuclear Services, ANSWERS/WIMS(99)9
7) B.J. Toppel, "A user's guide for the REBUS-3 fuel analysis capability", ANL-83-2, Argonne National Laboratory (1983)
8) J.A. Hendriks et al., "Neutronics validation during conversion to LEU", Proc. PHYSOR-20064)
9) E.Z. Müller et al., *Development of a Core Follow Calculational System for Research Reactors*, 9th Pacific Basin Nuclear Conference, Sydney, Australia, May 1-6-1994