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Generation of a Broad-Group HTGR Library for Use with SCALE

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Generation of a Broad-Group HTGR Library for Use with SCALE

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ABSTRACT

With current and ongoing interest in high temperature gas reactors (HTGRs), the U.S. Nuclear Regulatory Commission (NRC) anticipates the need for nuclear data libraries appropriate for use in applications for modeling, assessing, and analyzing HTGR reactor physics and operating behavior. The objective of this work was to develop a broad-group library suitable for production analyses with SCALE for HTGR applications. Several interim libraries were generated from SCALE fine-group 238- and 999-group libraries, and the final broad-group library was created from Evaluated Nuclear Data File/B Version ENDF/B-VII Release 0 cross-section evaluations using new ORNL methodologies with AMPX, SCALE, and other codes. Furthermore, intermediate resonance (IR) methods were applied to the HTGR broad-group library, and lambda factors and f-factors were incorporated into the library's nuclear data files. A new version of the SCALE BONAMI module named BONAMI-IR was developed to process the IR data in the new library and, thus, eliminate the need for the CENTRM/PMC modules for resonance self-shielding. This report documents the development of the HTGR broad-group nuclear data library and the results of test and benchmark calculations using the new library with SCALE. The 81-group library is shown to model HTGR cases with similar accuracy to the SCALE 238-group library but with significantly faster computational times due to the reduced number of energy groups and the use of BONAMI-IR instead of BONAMI/CENTRM/PMC for resonance self-shielding calculations.

FOREWORD

In recognizing the need for nuclear data appropriate for HTGR applications, a robust and versatile broad-group nuclear data library for use with SCALE was generated for the U.S. Nuclear Regulatory Commission. An HTGR-appropriate 81-group energy structure was selected with energy boundaries that are a subset of the standard SCALE 238-group structure. This nuclear data library is intended for HTGR applications. The final broad-group library was generated directly from ENDF/B-VII files using the latest methodology, and the intermediate resonance parameters, lambda factors and f-factors for important nuclides were included in the new library.

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ACRONYMS AND ABBREVIATIONS

1-D	one dimensional
2-D	two dimensional
3-D	three dimensional
AMPX	Analytical Methods Nuclear Cross-Section Processing Computer Code System
ASME	American Society of Mechanical Engineers
CE	continuous energy
CENTRM	Continuous Energy Transport Module
DCS	data control system
ENDF	evaluated nuclear data file
ENDF/B-VII.0	evaluated nuclear data file version VII
HTGR	high temperature gas reactor
HTR	high temperature reactor
HTS	heat transport system
HTTR	High Temperature Engineering Test Reactor
HX	heat exchanger
IR	intermediate resonance
LWR	light-water reactor
MOC	method of characteristics
MWd/te U	megawatt-days per metric ton of uranium
MWt	megawatt thermal
NGNP	next generation nuclear plant
NPP	nuclear power plant
NR	narrow resonance
NRC	U.S. Nuclear Regulatory Commission
OE	operating experience
ORNL	Oak Ridge National Laboratory
P&IC	pressure and inventory control
PBR	pebble bed reactor
pcm	parts per hundred thousand (cent mille)
PSA	probabilistic safety assessment
PW	pointwise
PWR	pressurized water reactor
RB	reactor building
RG	regulatory guide
SAS1X	SCALE Shielding Analysis Sequence 1X
SDC	shutdown cooling
SF	spent fuel
VHTR	very high temperature reactor
WR	wide resonance
XML	extensible markup language

1. INTRODUCTION

Analyses and simulations for high temperature gas reactor (HTGR) models require appropriate nuclear data libraries. In order to perform timely production calculations, a suitable broad-group neutron energy structure is required. Calculations using the broad-group library need to provide results comparable to calculations performed with fine-group libraries or continuous energy calculations.

Until now, most broad-group libraries have been prepared or generated with the intention of being suitable for light water reactors (LWRs). In this work, it is the goal to generate a broad-group nuclear data library for use in the Oak Ridge National Laboratory (ORNL) SCALE code system [1,2] for HTGR applications. Several broad-group HTGR cross-section libraries were produced with SCALE modules (e.g. MALOCS) or through the use of AMPX [3,4] modules. The selection of a suitable broad-group neutron energy structure resulted from analysis and assessment of HTGR neutron spectra and features of neutron resonances and reactions. The final HTGR 81-group library produced in this work was generated directly from ENDF/B-VII nuclear data files using ORNL library generation techniques and procedures. In addition, intermediate resonance (IR) treatment methods were applied to generate intermediate resonance (IR) parameters (including lambda factors and f-factors) that were added to the library. Furthermore, some additions and augmentations were made to the SCALE code software (in particular, BONAMI-IR) to implement the capability to utilize the IR parameters. The 81-group library is expected to be released in SCALE 6.2.

This report provides details of the process in which the broad-group structure of neutron energy group boundaries was determined. In addition, testing of model scenarios and benchmark calculations were completed using SCALE for a range of representative HTGR-related models. The results from SCALE calculations using the new HTGR broad-group libraries were compared with similar calculations using fine-group and ultra fine-group libraries and also with continuous energy KENO and MCNP [5] model results.

2. PROCEDURES AND METHODOLOGY FOR GENERATING HTGR LIBRARIES

The methodology for producing a broad-group nuclear data library for HTGR applications in SCALE modeling and simulation utilized AMPX and SCALE software modules in conjunction with analysis and interpretation of calculated relevant neutron spectra.

2.1 INTRODUCTION TO LIBRARIES

For this work, the main goal was to create an efficient and effective broad-group nuclear data library that would be suitable for use with SCALE HTGR models for production cases ranging from room temperature to 2000 K. The standard SCALE ENDF/B-VII cross-section library for reactor analysis contains 238 neutron energy groups. Recently, a fine-group library was generated, using a HTGR weighting function, with nuclear data in 999 neutron energy groups. An HTGR broad-group library with 81 energy groups was produced from this 999-group library. The libraries discussed in this report are all based on ENDF/B-VII nuclear data files.

2.2 ISSUES RELATED TO HTGR NEUTRONICS AND NUCLEAR DATA

HTGRs operate under conditions quite different from LWRs and pressurized heavy water reactors (PHWRs) for which many nuclear data libraries have been generated. The nuclear data libraries for HTGRs generally need to be suitable for the higher temperatures and characteristic neutron flux spectra that are generated in these reactors. There are special neutron resonances and material concerns associated with HTGR neutronics. Usually, fine group structure is needed in the nuclear data libraries so that all the neutron absorption, capture, and fission processes are appropriately simulated.

In order to generate a broad-group nuclear data library suitable for HTGR models, careful establishment of neutron energy boundaries is required such that major resonances and reactions will be treated properly. Various broad-group neutron energy structures were considered and assessed in this work, with reference to earlier broad multigroup libraries. The results of SCALE model scenarios with broad-group nuclear data libraries were compared against cases utilizing fine-group SCALE nuclear data libraries (238 and 999 groups). These cases were also compared against MCNP and KENO continuous energy simulations to assess the appropriateness of the broad-group libraries.

2.3 CODES AND TECHNIQUES

SCALE was used in this work in conjunction with AMPX [3,4] and other nuclear data codes, such as RIML [8]. Monte Carlo calculations with MCNP and SCALE/KENO were used in addition to deterministic neutron transport simulations. Representative HTGR pin cell and full core models were analyzed. Furthermore, a series of HTGR benchmark model scenarios were assessed with the different nuclear data libraries to test the suitability of the newly generated broad-group nuclear data libraries. In addition to using ENDF/B-VII data files with appropriate weighting functions to generate broad-group nuclear data for use with HTGRs, appropriate nuclide-dependent Bondarenko IR f-factors and lambda factors were implemented with the nuclear data. Necessary modifications to implement the IR methodology in SCALE were performed and used in the analyses.

2.3.1 RIML

RIML [8] is a code for generating IR parameters, self-shielded cross sections, subgroup levels and weights, and the associated AMPX master libraries. RIML is a control module composed of three separate programs: RILAMB, IRVING, and SUBGR. RILAMB generates IR parameters for the homogeneous mixtures and self-shielded cross sections as a function of background cross section for the homogeneous and heterogeneous geometries. Self-shielded cross sections are converted into the Bondarenko factors and into the resonance integral table. IR parameters and Bondarenko factors are to be included or replaced in the master AMPX library using IRVING. SUBGR uses the resonance integral table created by RILAMB to generate the subgroup levels and weights. These subgroup data can be used in a transport lattice code, such as DeCART, which uses the subgroup method to self-shield resonance group cross sections.

The wide and the narrow resonance (NR) approximations have been combined [10], together forming an IR approximation that is good for the resonance range from a few electron volts up to 100 keV. IR parameters can be used to interpolate between the narrow and wide resonance approaches. Because nearly all deterministic transport codes use multigroup cross sections, utilizing between 30 and 300 groups, it is very important to use the appropriate approximations to estimate the effective group self-shielded cross section.

Many kinds of methods have been developed for the resonance treatment in this energy range. However, in many cases the basic approach for the resonance treatment is similar. The self-shielded cross sections are tabularized in advance as a function of some parameter such as background cross section by using various methods. One of the typical methods is to obtain the self-shielded cross sections by solving the continuous or ultrafine group slowing-down equation and to obtain the corresponding background cross section to complete the self-shielded cross-section table.

The CENTRM/PMC codes are used to estimate the self-shielded group cross sections by solving the slowing-down equation with the continuous energy cross sections and integrating the continuous energy flux and cross section over each group. These effective self-shielded group cross sections are used in SCALE multigroup/transport codes (e.g. NEWT, KENO) directly. The SCALE CENTRM/PMC codes can be used to obtain the self-shielded group cross-section table through a slight modification and a combination with a module to generate the corresponding background cross section.

The program RILAMB (Resonance Integral and Lambda) has been developed to compute IR parameters and self-shielded cross-section tables using the results from CENTRM/PMC in the SCALE system. IR parameters are generated for a set of homogeneous mixtures, and self-shielded group cross-section tables are generated for the specified homogeneous and heterogeneous geometries. The program IRVING uses the self-shielded cross-section tables to generate Bondarenko factors and resonance integral tables. IRVING replaces the original NR Bondarenko factors in the master AMPX library and adds the IR parameters.

2.3.2 Creating a Multigroup Library

A flow diagram is presented in Figure 2.1 to illustrate the automated procedure to generate the AMPX master library from ENDF/B evaluations.

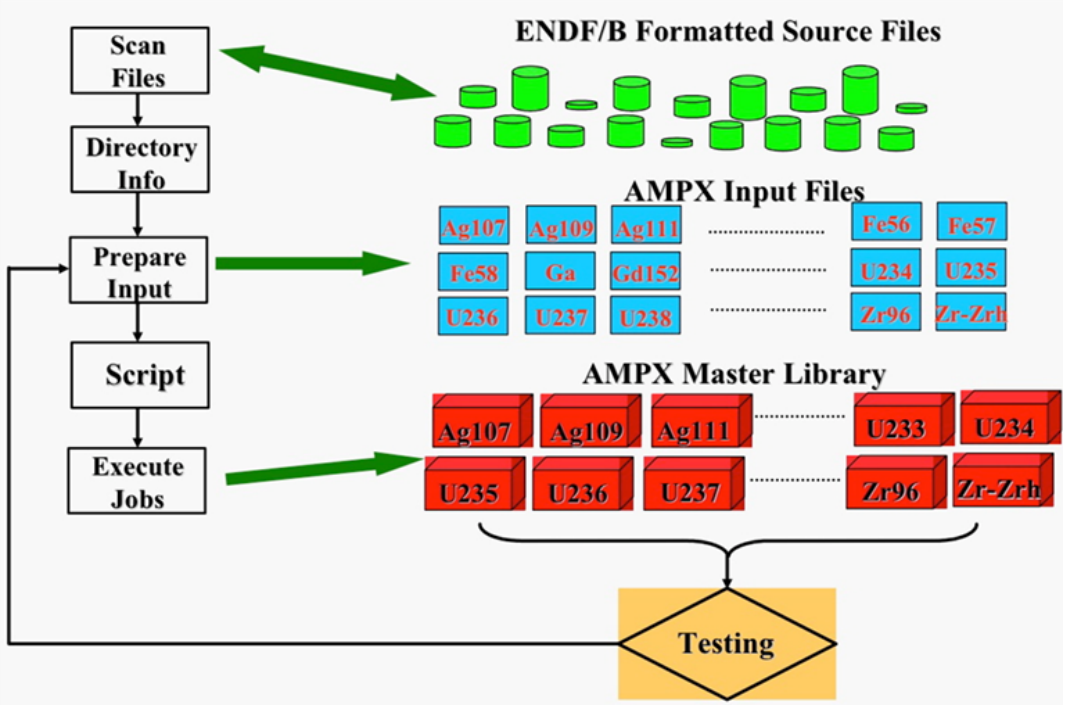

Figure 2.1. Work flow for AMPX master library creation.

2.4 GENERATION OF LIBRARIES FROM ENDF/B-VII FILES

In this ORNL process, the input files are generated automatically using extensible markup language (XML) templates. The general flow of creating the nuclear data in this methodology is depicted in Figure 2.2. The AMPX modules and utility codes employed in this process are described below and shown in the flowchart.

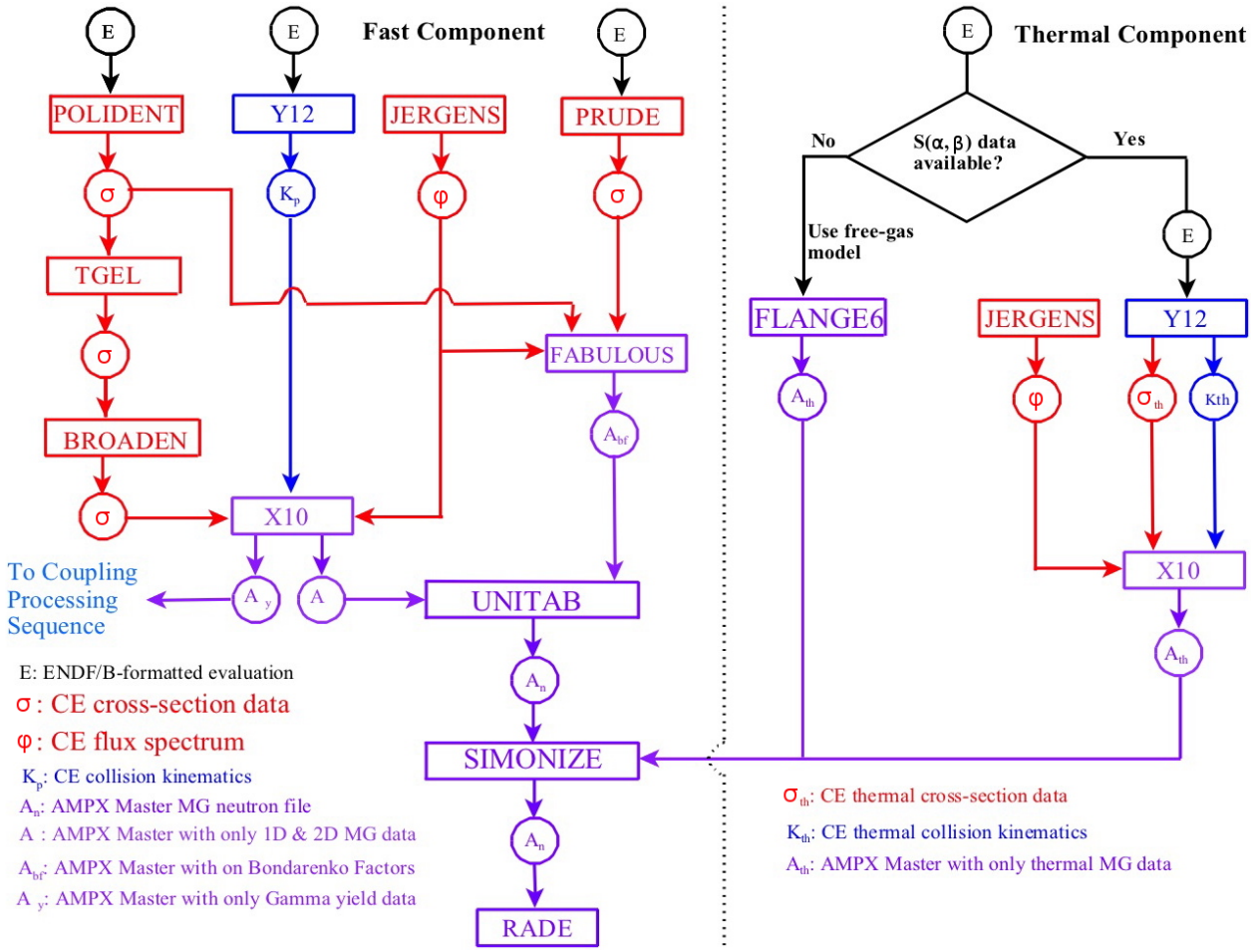

Figure 2.2. AMPX sequence for producing neutron multigroup data.

The following AMPX modules are used in the process to produce a neutron multigroup library.

POLIDENT: Creates pointwise cross-section data at 0 K from the ENDF/B-VII data files. For resonance nuclides, POLIDENT contains a procedure that determines a point energy mesh in the resolved resonance region and calculates the cross sections on that energy mesh. The pointwise data are stored as x-y values on a linear-linear grid.

TGEL: When all of the cross-section data are produced on a linear-linear grid, the sum of a group of linear functions is itself linear; however, simply linearizing the data that are given in an evaluation does not lead to this consistency. To ensure consistency, the total cross section and other "redundant" reactions (e.g., fission, inelastic) are formed by summing the partial values. This module is used to ensure that all redundant reactions are equal to the sum of the partial reactions.

BROADEN: This module is used to Doppler broaden the cross-section data.

PRUDE: For nuclides with unresolved resonance data, this module is run to produce point averaged cross sections that are a function of temperature and background cross section (background cross sections are discussed in more detail in Section 2.5). The background cross section is simply defined as the cross section per unit atom of a nuclide of the mixture (other than the nuclide itself) in which the nuclide

is mixed. In the sequences that were prepared, temperatures of 293, 900, and 2100 K were chosen, along with background values of 10^{-6}, 1, 10, 100, 1000, 10^4, 10^5, 10^6, and 10^8 barns.

FABULOUS: For all nuclides, the point data from PRUDE (if applicable) and POLIDENT are passed to this module with the weighting spectrum file. FABULOUS uses the same temperatures and background cross sections described for PRUDE to numerically Doppler broaden the functions exterior to the unresolved region, after which the functions are spliced together with the appropriate unresolved functions. These spliced functions are then used in a numerical scheme that calculates Bondarenko factors for all nuclides for elastic scattering, capture, fission, and total cross sections.

UNITAB and SIMONIZE: These modules are used to combine partial master libraries generated by FLANGE6, FABULOUS, and X10 into a cohesive AMPX MG master library for a given evaluation. The module combines the data into one AMPX MG master library after recalculating and renormalizing the data.

JERGENS: This module is used to generate the flux used to collapse point-wise data to MG format.

Y12: This module reads an ENDF/B evaluation and produces tabular double-differential collision kinematics data for all reactions. The functions it produces tell what particles are produced and at what energies and directions when a reaction is encountered at some source energy point. The output from Y12 is an AMPX tabular kinematics file.

X10: The weighting spectrum, the point data from BROADEN, and the kinematics data from Y12 are passed to X10. X10 produces a group-averaged AMPX master library.

FLANGE6: This module is used to produce thermal scattering matrices at 293, 600, 900, 1200, and 2100 K based on the free-gas scattering model.

RADE: This module is used to perform internal consistency checks on the AMPX master library.

To generate the 999-group library, we used the AMPX JERGENS module to generate a smooth weighting spectrum that has the form of a Maxwellian–1/E–fission spectrum–1/E above 10 MeV. For the 81-group library 81B3 and 81C, we used a custom flux as the weighting function. Figure 2.3 shows the pointwise flux generated in CENTRM (from the HTGR prismatic fuel SCALE input case listed in Appendix C) for two representative temperatures. The pointwise flux data (approximately 16,000 data points) at a temperature of 1800 K was chosen to be the weighting function for the generation from the ENDF/B-VII nuclear data files [11] of the 81-group library.

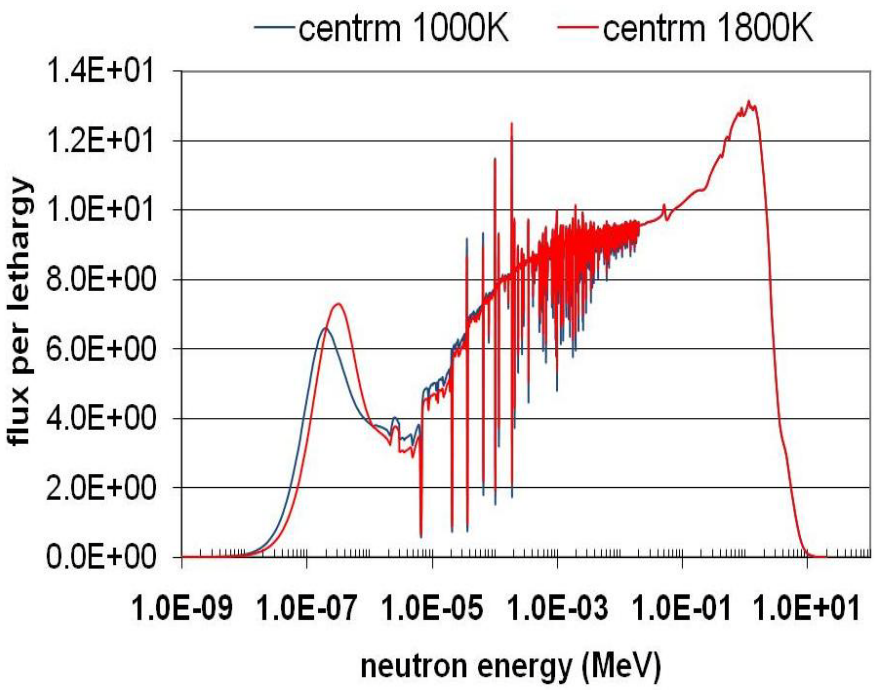

Figure 2.3. Comparison of CENTRM pointwise flux weighting functions for the HTGR temperatures.

2.5 INTERMEDIATE RESONANCE CONSIDERATIONS

This section is a summary of the new methods and data that were added as an IR treatment in the new library. The resonance data in SCALE 6.1 and all earlier versions of SCALE were based on the neutron spectrum from the narrow resonance approximation. With the new IR methods applied for selected isotopes (e.g., ^{238}U), new Bondarenko factor tables were generated based on a more rigorous neutron flux spectrum. In addition, IR parameters (lambda factors) have been added for the evaluation of background cross sections in the resonance treatment with the IR approximation.

2.5.1 IR method

The effective shielded cross section in a resonance group g can be written [10] as

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x(u)\phi(u)du}{\int_{\Delta u_g} \phi(u)du}.$$

where $\emptyset$ = flux and u = lethargy.

In the narrow resonance (NR) approach, the neutron spectrum is simply inversely proportional to the total cross section:

$$\phi(u) = \frac{\text{constant}}{\Sigma_t(u)}.$$

In a more sophisticated IR method, the flux spectrum can be written as

$$\phi(u) = \frac{\sigma_b}{\sigma_a(u) + \sigma_b}$$

where a background cross section is defined as

$$\sigma_b = \frac{1}{N_r} \sum_{i=all} N_i \lambda_i \sigma_{p,i} ,$$

N_r is the atomic number density of the resonance nuclide, N_i is the atomic number density of isotope *i*, λ_i is the IR parameter of isotope *i*, and $\sigma_{p,i}$ is the potential cross section of isotope *i*. In case of heterogeneous problems, the background cross section can be adjusted as below using the equivalence theory:

$$\sigma_b \rightarrow \sigma_b + \sigma_e$$

where σ_e is the escape cross section,

$$\sigma_e = \frac{1}{N_r} \frac{a(1-c)}{\bar{l}} ,$$

in which *a* is the Bell factor, *c* is the Dancoff factor, and $\bar{l}$ is the mean chord length of fuel region.

2.5.2 Library generation

As shown above, in order to apply the IR method, the resonance integrals of isotopes selected for IR treatment need to be recalculated either by using the IR definition of flux spectrum or using a neutron slowing-down solver such as CENTRM. The lambda factors also need to be generated for implementation in a new library to allow for the application of the IR method in the BONAMI-IR module in SCALE.

New Bondarenko factors

The Bondarenko factors of given resonance materials are computed using a pointwise (PW) flux spectrum for an infinite homogeneous mixture of the resonance nuclide combined with hydrogen. The hydrogen concentration in the mixture is varied to obtain the desired σ_b values corresponding to different degrees of self-shielding for the particular resonance material. The temperature of the resonance material is also varied to account for the impact of Doppler broadening on self-shielding. CENTRM was used to calculate the PW flux in the homogeneous media for each hydrogen concentration (i.e., σ_b) and resonance Doppler temperature, for each resonance nuclide of interest. PMC was used to compute the corresponding self-shielded cross sections. The Bondarenko factor is the ratio of the self-shielded cross section from PMC divided by the infinitely dilute (unshielded) cross section in the library. For example in the case of ^{238}U, CENTRM/PMC was run for three Doppler temperatures of 293, 900, and 2000 K and 93 different hydrogen concentrations. This corresponds to 3 X 93 = 279 CENTRM/PMC cases. The Bondarenko factors at the desired background cross section values (σ_b) in the library were interpolated from these results. Table 2.1 shows the final background cross section values for which ^{238}U Bondarenko factors are tabulated in the library. The Bondarenko factors for other resonance materials were generated similarly, but different hydrogen concentrations may have been used.

Table 2.1. Background cross sections for Bondarenko factors of ^{238}U

Background cross section (barns)	Background cross section (barns)	Background cross section (barns)
1.00E-06	1.20E+02	1.00E+05
1.00E+00	1.60E+02	1.00E+08
1.00E+01	3.20E+02	
1.50E+01	6.40E+02	
2.00E+01	1.00E+03	
3.00E+01	2.00E+03	
4.00E+01	5.00E+03	
6.00E+01	1.00E+04	
8.00E+01	2.00E+04	

From the CENTRM/PMC outputs of these cases, the effective cross sections of ^{238}U have been collected and converted to Bondarenko factor tables using the following definition:

$$f_{x,g}(T_f,\sigma_b) = \frac{\sigma_{x,g,eff}(T_f,\sigma_b)}{\sigma_{x,g,\infty}},$$

where f is the Bondarenko factor, T_f is the fuel temperature, $\sigma_{x,g,eff}$ is the effective cross section of type x, and $\sigma_{x,g,\infty}$ is the infinitely dilute cross section. These factors have been tabulated in the library at three temperatures (293, 900, and 2000 K) and 19 background cross sections (1×10^{-6}, 10, 15, 20, 30, 40, 60, 80, 120, 160, 320, 640, 1000, 2000, 5000, 10,000, 20,000, 1×10^6, and 1×10^8 barns). Before this modification to the process, the original library had Bondarenko factors for only nine background cross sections.

Lambda factors

Lambda factors are also called hydrogen equivalence parameters and are calculated in the following procedure:

1) Compute a $\sigma_{a,g}^{238}$ table as a function of $\sigma_{b,g}^{238}$ by changing the particle number density of hydrogen for a homogeneous mixture at the fixed ^{238}U (N^{238}) particle number density. The calculation of the effective cross sections has been done in CENTRM/PMC and RIML has been used for the processing of the data.
2) Compute the slowing-down calculation for a mixture of ^{238}U (N^{238}), ^{1}H (N^{1}) and a target nuclide x (N^{x}), and obtain a new $\sigma_{a,g}^{238}$ (CENTRM/PMC).
3) Read the corresponding $\sigma_{b,g}^{238}$ from the prepared $\sigma_{a,g}^{238}$ table (RIML).
4) Calculate the hydrogen equivalence parameter of the isotope x using the following equation (RIML), where $\boldsymbol{\sigma_p}$ is the potential cross section (refer to Appendix A).

$$\lambda_g^x = \frac{\sigma_{b,g}^{238} N^{238} - N^{238}\lambda_g^{238}\sigma_p^{238} - N^1\lambda_g^1\sigma_p^1}{N^x\sigma_p^x}.$$

The above procedure has been applied to all the isotopes in the old library, and the calculated lambda factors have been added to a new library at MT=2000. The lambda factors have been generated for a single fuel temperature of 300K.

2.5.3 Library testing

A simple HTGR pin cell has been used for testing the implemented method. In the model, the fuel kernels in the compact have been homogenized with graphite. The calculated k-effective values are summarized in Table 2.2 as a function of pin pitches. The fuel temperature used for testing is 900 K to match the cross-section data for the continuous energy calculations with KENO. NR and IR results from XSDRN are compared with continuous energy KENO (CE KENO), which is considered the reference solution in lieu of measured data, and with CENTRM, which is the reference method for generating the IR factors. In other words, BONAMI-IR results cannot be expected to be better than the CENTRM results. Note that the large differences between NR and CENTRM/CE KENO are expected. They demonstrate the inadequacy of the NR methodology for thermal systems, which is the reason for developing the IR method.

The results presented in Table 2.2 and the following tables in this section are based on preliminary investigations in the development of the IR methodology. The calculated results for the final method in Section 4 provide validation of the 81-group library for real world HTGR applications.

Table 2.2. Assessing the IR-methods improvement to the library: HTR pin-cell test problem

Pitch (cm)	CE KENO	238-Group KENO							
		BONAMI-NR	Δk (pcm) vs. CE KENO	BONAMI-IR	Δk (pcm) vs. CE KENO	CENTRM (n2d=0,ibr=3)	Δk (pcm) vs. CE KENO	NR vs. CENTRM Δk (pcm)	IR vs. CENTRM Δk (pcm)
1.5	0.97725	1.17518	19793	0.97398	-327	0.97587	-138	19931	-189
2.0	1.21413	1.39732	18319	1.20669	-744	1.20919	-494	18813	-250
2.5	1.38634	1.53469	14835	1.37588	-1046	1.37967	-667	15502	-379

For the 238-group library, the nuclear data library with IR treatment is significantly improved over the old library with the NR approach.

2.6 TESTING OF BONAMI-IR DURING IMPLEMENTATION INTO SCALE

As part of the process of implementing IR treatment into BONAMI (also called BONAMI-IR), several comparisons were made between BONAMI-IR, standard BONAMI (BONAMI-NR), CENTRM, and continuous energy KENO. The BONAMI-IR calculations used a new IR-relevant 238-group library (238ir) that was generated using the HTGR CENTRM weighting function. The results presented in Tables 2.3–2.5 were calculated with XSDRN for an infinite homogeneous medium of very low enriched uranium (LEU) and hydrogen with different background cross sections. Table 2.6 presents results for a simplified PWR pin cell, and Table 2.7 compares results for a doubly heterogeneous HTGR pin cell. The agreement between the BONAMI-IR and the CE KENO results is generally on the same order as the CENTRM results and significantly better than that of BONAMI-NR, with the exception of Table 2.6. The discrepancy between MG KENO/CENTRM and CE KENO for LWR pin cells has been previously observed with the standard SCALE V7-238 library and is under investigation. Note that the BONAMI-IR and CENTRM results are consistent. The fact that the BONAMI-NR result is better for this case is most likely due to a cancellation of errors.

Table 2.3. Infinite homogeneous medium of 1.26% enriched LEU and H; background XS ~ 100 b and temperature 300K

Code	BONAMI method	MG XS library	Eigenvalue	Δk (pcm) Diff from CE KENO
CE KENO	–	–	1.09394 ± 0.00021	–
CENTRM	IR	238ir	1.09508	114
BONAMI	IR	238ir	1.09648	254
BONAMI	NR	238	1.10282	888

Table 2.4. Infinite homogeneous medium of 1.26% enriched LEU and H; background XS ~ 50 b and temperature 300K

Code	BONAMI method	MG XS library	Eigenvalue	Δk (pcm) Diff from CE KENO
CE KENO	–	–	1.05673 ± 0.00019	–
CENTRM	IR	238ir	1.05855	182
BONAMI	IR	238ir	1.05560	-113
BONAMI	NR	238	1.06525	852

Table 2.5. Infinite homogeneous medium of 1.26% enriched LEU and H; background XS ~ 25 b

Code	BONAMI method	MG XS library	Eigenvalue	Δk (pcm) Diff from CE KENO
CE KENO	–	–	0.95583 ± 0.00020	–
CENTRM	IR	238ir	0.95861	278
BONAMI	IR	238ir	0.95812	229
BONAMI	NR	238	0.96553	970

Table 2.6. Simplified PWR pin cell 3.34% enriched UO_2, pitch = 1.44 cm; pellet OR = 1.44 cm; Temperature 300K

Code	BONAMI method	MG XS library	Eigenvalue	Δk (pcm) Diff from CE KENO
CE KENO	–	–	1.35578 ± 0.00022	–
MG KENO/CENTRM	IR	238ir	1.34903 ± 0.00018	-675
MG KENO/BONAMI-IR	IR	238ir	1.34714 ± 0.00019	-864
BONAMI/ XSDRN	NR	238	1.34948	-630

Table 2.7. Double-het HTR pin cell and temperature 300K

Code	MG XS library	Eigenvalue	Δk (pcm) Diff from CENTRM double-het
XSDRN/CENTRM	238ir	1.29596	–
XSDRN/BONAMI-IR	238ir	1.29797	201

2.7 SUMMARY OF LIBRARY GENERATION METHODS

Several methods of nuclear data library generation were employed in this work. The MALOCS utility module in SCALE was used to condense existing SCALE nuclear data libraries into appropriate broad-group energy structures using HTGR case-calculated weighting functions (based on case neutron flux distributions). This procedure was used in the creation of the interim broad-group libraries 81A, 81B, and 81B2. The other major methodology for creation of a nuclear data library is to generate it directly from ENDF/B data files, using continuous energy (pointwise) weighting functions, such as generated with CENTRM. This process was used to generate the recent 999-group library for SCALE (with independent weighting function) and was used in generating a new IR-relevant 238-group library using the HTGR CENTRM weighting function. The 81B3 broad-group library was also generated in this manner, using the neutron energy group structure of 81B2, but with the CENTRM generated weighting function rather than the neutron flux from 999- and 238-group SCALE HTGR model calculations.

To provide additional computational efficiency by removing the need to use CENTRM/PMC for unit cell calculations, the final broad-group libraries were enhanced and augmented with IR lambda factors and f-factors. These IR-enhanced nuclear data libraries were used in case calculations for HTGR models using a developmental version of SCALE in which the new IR features can be accessed and used in cases as discussed in the following section.

3. NUCLEAR DATA LIBRARIES

3.1 INTRODUCTION

The SCALE 6.1 code system includes both pointwise (PW) and multigroup (MG) libraries processed from ENDF/B-VII nuclear data files using SCALE and the AMPX code system. The PW data are used for two distinct functions in SCALE. First, they are used for three-dimensional (3D) continuous-energy (CE) Monte Carlo calculations with KENO. Second, they are used in the one-dimensional (1-D) CENTRM CE discrete ordinates code to compute pointwise flux spectra for generating self-shielded MG cross sections. The PW nuclear data are stored on a very fine energy mesh so that the value at any energy can be linearly interpolated with an error of less than 0.1%.

Figure 3.1 presents a comparison of neutron spectra calculated with SCALE for a representative HTGR homogeneous prismatic fuel model case input, "vhtr" (listed in Appendix B), using a 999-group ENDF/B-VII library at three different representative temperatures of 300 K, 900 K, and 1700 K. In addition, the 999-group HTGR neutron spectrum at 1700 K is compared with a 238-group spectrum at the same temperature in Figure 3.2. The 238-group ENDF/B-VII library is the most current and generally recommended library in SCALE 6.1. The 999-group library has been developed and used internally at ORNL for various studies [6]. This 999-group library allows calculations to be performed with an ultra fine neutron energy mesh, allowing multigroup calculations that more closely resemble continuous energy representations. Note that the 238-group structure is a subset of the 999-group structure, i.e., the boundaries of the 238-group structure align with boundaries in the 999-group structure.

Figure 3.2 compares the 238-group and the 999-group neutron flux spectra calculated for the SCALE vhtr input model (listed in Appendix B) at a temperature of 1700K. As seen in the figure, the spectra are very similar for the main characteristics. However, the 999-group spectra, by virtue of its near-continuous energy fine group aspects shows more detail and structure in the resolved and unresolved resonance regions.

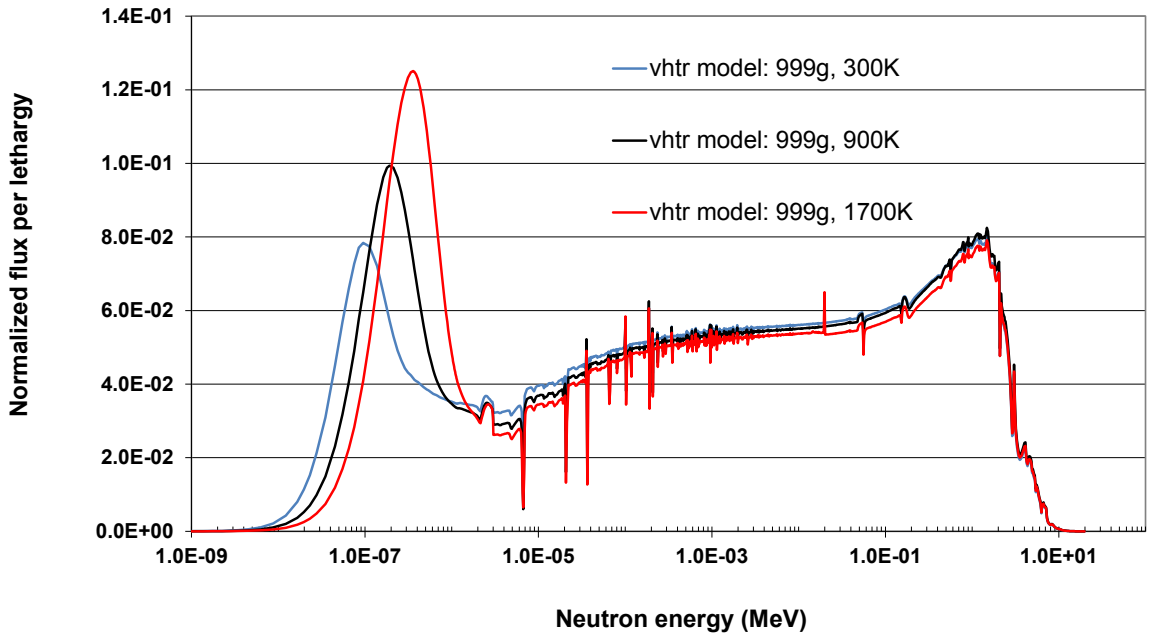

Figure 3.1. Comparison of HTGR spectra in 999-group calculations for a range of temperatures.

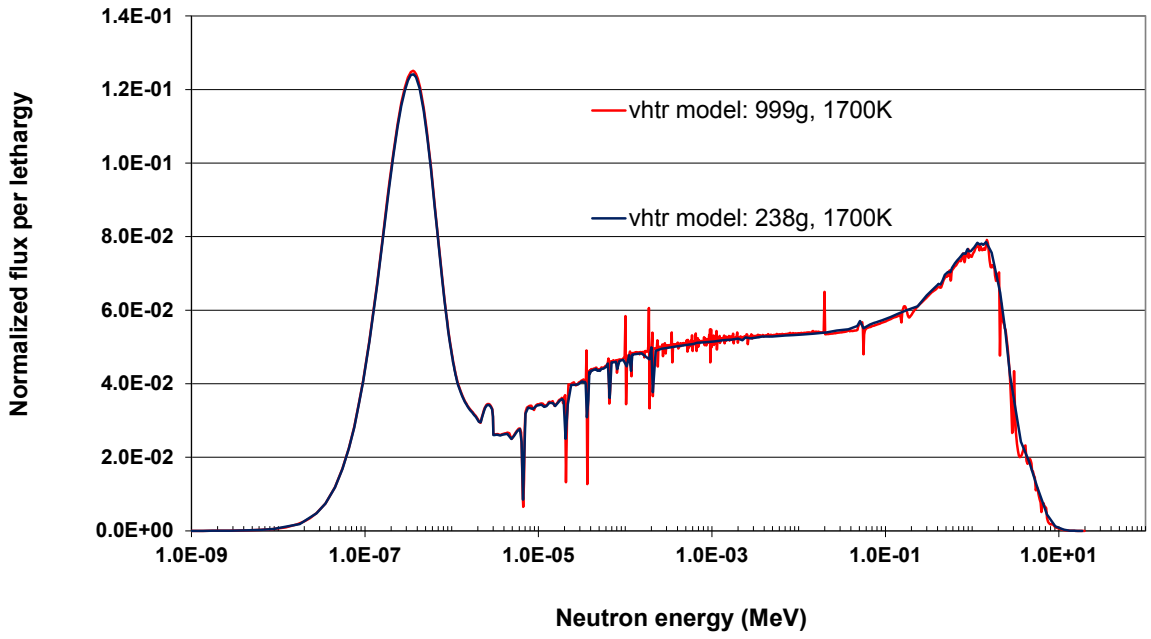

Figure 3.2. Comparison of HTGR spectra in 238- and 999-group calculations.

In this report, neutron flux spectra are plotted in two ways, with the y-axis for both methods representing the neutron flux level divided by the lethargy of the energy group bins (the natural log of the ratio of the bin upper energy to the bin lower energy). The first plotting method (used in Figure 3.1) plots the flux per unit lethargy against the average bin neutron energy. The other plotting method is to use histograms for the full neutron energy bin with each bin ranging from its lower to higher neutron energy limits.

Figure 3.3 provides more detail of the neutron spectra calculated with SCALE using 238- and 999-group nuclear data libraries in Figure 3.2 over the energy range of 1 to 10 eV, which includes the large neutron capture resonance at 6.7 eV for ^{238}U reactions. The agreement in this large neutron capture resonance between the 238-group and the 999-group neutron flux representations with SCALE is quite good for HTGR simulation cases. Small differences are evident between the solutions due to the much finer neutron energy group structure in the 999-group nuclear data library. Note that the broad peak between 2 to 3 eV in this and other figures is not physical. It is caused by truncation of the thermal scattering at 3 eV in the SCALE multigroup (MG) libraries. This phenomenon is more noticeable for graphite. The impact on calculations is typically negligible, because there are no important resonances at this energy. The SCALE team has plans to address this problem in the near future.

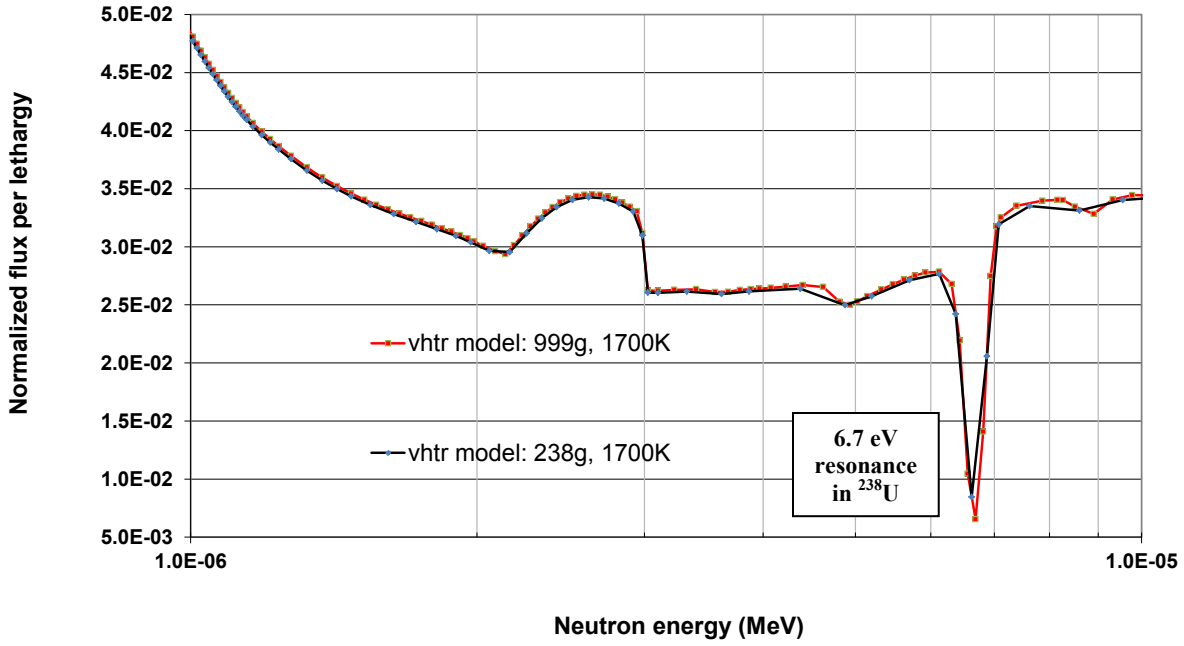

Figure 3.3. Comparison of HTGR spectra (238 group and 999 group) in the 1 to 10 eV region.

3.2 GENERATING BROAD-GROUP LIBRARIES

In this project, a number of interim broad-group nuclear data libraries were generated in 81 neutron energy groups; a previous study of the efficacy of nuclear data libraries for use in modeling VHTRs considered broad-group libraries with 72 and 79 groups [7]. Several broad-group neutron energy structures were devised by adding several judiciously placed energy bins to the library energy structure starting with that of the 72-group structure. The first 81-group broad-group library (81A) was a subset of the 999-group ultra fine group library with the neutron energy boundaries selected to capture the important resonances and features in the HTGR spectrum. The second broad-group structure (81B3) was established by shifting energy group boundaries in 81A that did not align with the 238-group structure so that the energy boundaries in 81B are a subset of the standard SCALE fine-group 238-group library energy bin boundaries.

Figure 3.4 compares the fine detail in the 238- and 999-group flux solutions for the HTGR prismatic fuel case for the 10 to 100 eV neutron energy range in the spectra. As can be seen, the 999-group flux solution shows deeper flux dips in the narrow resonances followed by increases in flux level at the lower energy side of the resonances, which is consistent with the somewhat reduced cross section that would be in effect. This is clearly evident for the 36 eV (3.6×10^{-5} MeV) neutron resonance region seen in the middle of Fig. 3.4.

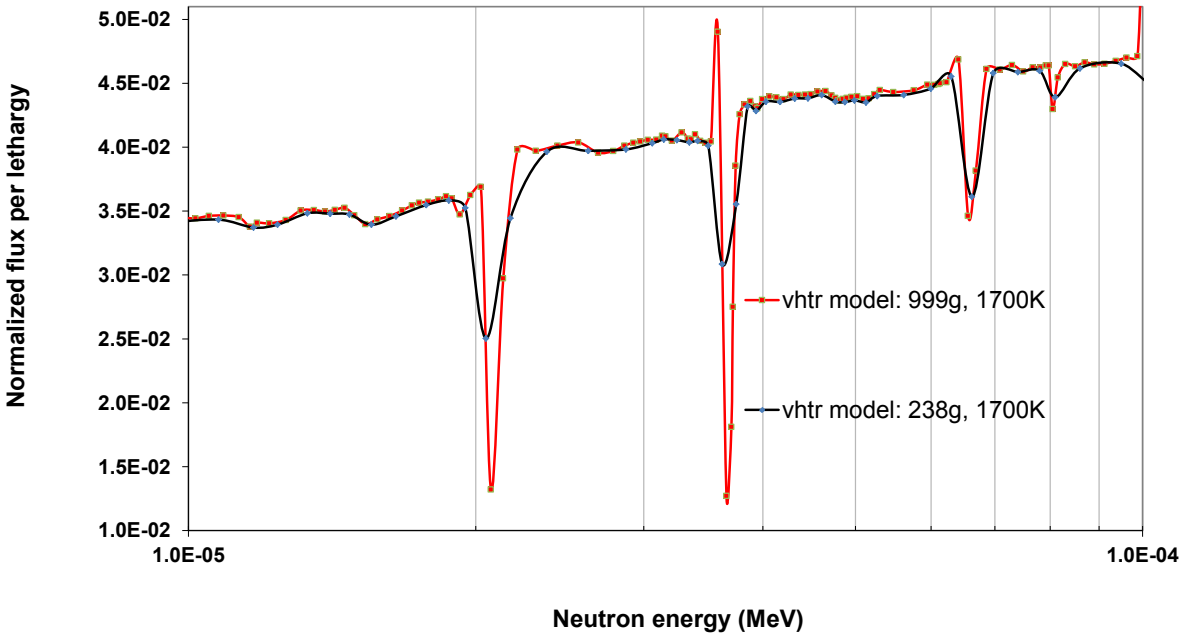

Figure 3.4. HTGR spectra in the 10 to 100 eV region: comparison of fine-group solutions.

In Figure 3.5, histograms representing the 81 group neutron flux spectra solutions for the 81A and 81B3 nuclear data libraries in the 10 to 100 eV neutron energy range are displayed in addition to the spectra from Fig. 3.4 to show the applicability of the chosen group energy structures to the resonances and details of the calculated multigroup neutron spectra.

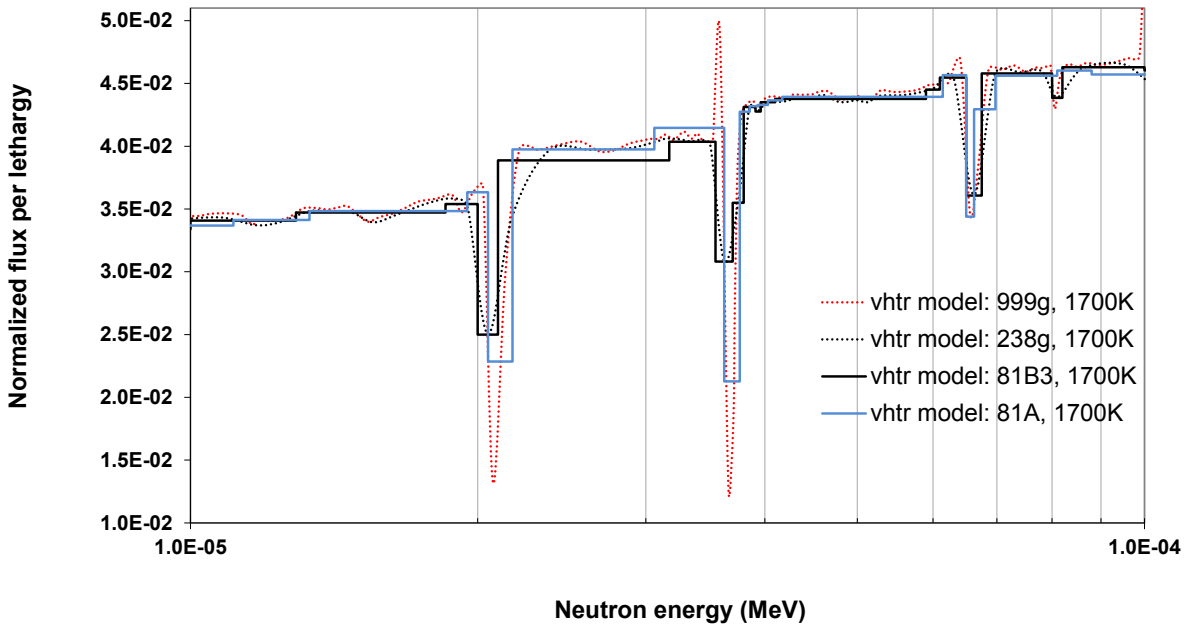

Figure 3.5. HTGR spectra in the 10 to 100 eV range for broad and fine group libraries.

Recall that the energy structure in library 81A is a subset of the 999-group library energy structure, while the 81B3 energy structure is a subset of the 238-group SCALE fine-group library (which is also a subset of the 999-group library). As would be expected, the flux dips in the 81A spectrum agree more closely with the 999-group spectrum while the 81B3 spectrum is similar to the 238-group spectrum. The comparison in Figure 3.5 is illustrated in a different way in Figure 3.6 by using a fine-group histogram for the 999-group solution in the 10 to 100 eV range.

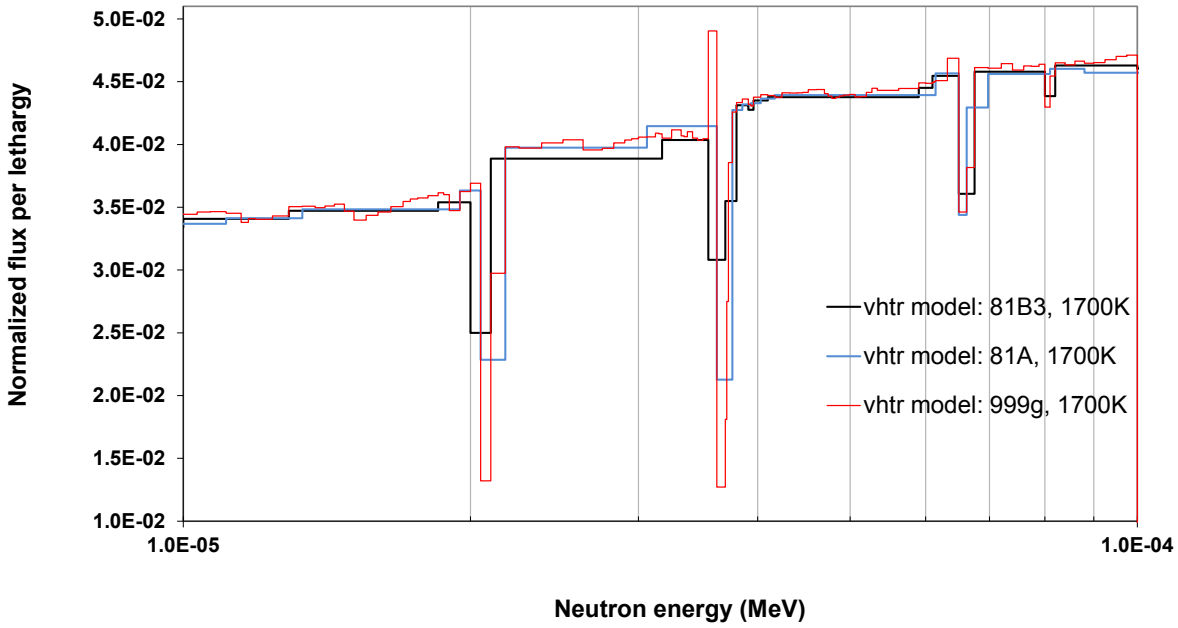

Figure 3.6. HTGR 238-group spectrum in the 10 to 100 eV region: broad-group comparisons.

In Figure 3.6 the 999-group fine-group spectrum plotted in histogram format shows the details also seen in the curves in Figs. 3.4 and 3.5. Although differences can be seen between the 81A and 81B3 spectra, the energy boundaries for both 81-group libraries are adequately positioned to address the major HTGR-related resonances for prismatic and pebble bed fuels.

3.3 DESCRIPTION OF THE BROAD-GROUP LIBRARIES

3.3.1 Library 81A

Library 81A was developed by condensing the new 999-group library with the SCALE module MALOCS using a 999-group neutron flux solution as a weighting function. The neutron-energy structure for 81A was selected from the available 999 neutron energy group boundaries, with care taken to select boundaries that surround major resonances and neutron spectrum features for HTGRs. Table 3.1 compares the energy group boundaries for the 999-group, the 238-group, and the various 81-group libraries.

Table 3.1. Neutron energy group structure comparisons for 999-, 238-, and 81-group

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
2.000E+07	1	1	1	1
1.964E+07	2			
1.900E+07	3			
1.845E+07	4			
1.790E+07	5			
1.733E+07	6	2		
1.691E+07	7			
1.649E+07	8			
1.608E+07	9			
1.568E+07	10	3		
1.530E+07	11			
1.492E+07	12			
1.455E+07	13	4		
1.419E+07	14			
1.384E+07	15	5		
1.350E+07	16			
1.317E+07	17			
1.284E+07	18	6		
1.252E+07	19			
1.221E+07	20			
1.191E+07	21			
1.162E+07	22			
1.133E+07	23			
1.105E+07	24			
1.078E+07	25			
1.051E+07	26			
1.025E+07	27			
1.000E+07	28	7		
9.753E+06	29		2	
9.512E+06	30			
9.278E+06	31			
9.048E+06	32			
8.825E+06	33			
8.607E+06	34			
8.395E+06	35			
8.187E+06	36	8		2
7.985E+06	37		3	
7.788E+06	38			
7.596E+06	39			
7.408E+06	40			
7.225E+06	41			
7.047E+06	42			
6.873E+06	43			
6.703E+06	44			
6.592E+06	45			
6.434E+06	46	9		3
6.376E+06	47		4	
6.219E+06	48			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
6.065E+06	49			
5.916E+06	50			
5.770E+06	51			
5.627E+06	52			
5.488E+06	53			
5.353E+06	54			
5.221E+06	55			
5.092E+06	56			
4.966E+06	57			
4.882E+06	58			
4.800E+06	59	10		4
4.724E+06	60			
4.607E+06	61			
4.493E+06	62			
4.398E+06	63			
4.304E+06	64	11		
4.183E+06	65		5	
4.066E+06	66			
3.965E+06	67			
3.867E+06	68			
3.772E+06	69			
3.679E+06	70			
3.588E+06	71			
3.499E+06	72			
3.413E+06	73			
3.329E+06	74			
3.247E+06	75			
3.166E+06	76			
3.080E+06	77			
3.000E+06	78	12		5
2.932E+06	79		6	
2.865E+06	80			
2.794E+06	81			
2.725E+06	82			
2.658E+06	83			
2.592E+06	84			
2.535E+06	85			
2.479E+06	86	13		6
2.466E+06	87		7	
2.385E+06	88			
2.365E+06	89			
2.354E+06	90	14		7
2.307E+06	91		8	
2.231E+06	92			
2.176E+06	93			
2.123E+06	94			
2.070E+06	95			
2.019E+06	96			
1.969E+06	97			
1.921E+06	98			
1.850E+06	99	15		8

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
1.827E+06	100			
1.782E+06	101			
1.738E+06	102			
1.695E+06	103			
1.653E+06	104			
1.612E+06	105			
1.572E+06	106			
1.536E+06	107			
1.500E+06	108	16		
1.461E+06	109		9	
1.423E+06	110			
1.400E+06	111	17		9
1.356E+06	112	18		
1.317E+06	113	19		
1.287E+06	114			
1.250E+06	115	20		
1.225E+06	116			
1.200E+06	117	21		
1.165E+06	118			
1.136E+06	119			
1.108E+06	120	22		
1.100E+06	121			
1.070E+06	122			
1.040E+06	123			
1.010E+06	124	23		
1.003E+06	125			
9.800E+05	126			
9.616E+05	127			
9.400E+05	128			
9.200E+05	129	24		
9.072E+05	130		10	
9.000E+05	131	25		10
8.874E+05	132			
8.750E+05	133	26		
8.611E+05	134	27		
8.506E+05	135			
8.403E+05	136			
8.301E+05	137			
8.200E+05	138	28		
8.100E+05	139			
8.002E+05	140			
7.904E+05	141			
7.808E+05	142			
7.730E+05	143			
7.653E+05	144			
7.576E+05	145			
7.500E+05	146	29		
7.427E+05	147			
7.335E+05	148			
7.244E+05	149			
7.154E+05	150			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
7.065E+05	151			
6.926E+05	152			
6.790E+05	153	30		
6.700E+05	154	31		
6.622E+05	155			
6.545E+05	156			
6.468E+05	157			
6.393E+05	158			
6.313E+05	159			
6.235E+05	160			
6.158E+05	161			
6.081E+05	162			
6.000E+05	163	32		
5.891E+05	164			
5.784E+05	165			
5.730E+05	166	33		
5.672E+05	167			
5.614E+05	168			
5.557E+05	169			
5.500E+05	170	34		
5.432E+05	171			
5.365E+05	172			
5.299E+05	173			
5.234E+05	174			
5.173E+05	175			
5.113E+05	176			
5.054E+05	177			
4.995E+05	178	35		
4.920E+05	179			
4.845E+05	180			
4.772E+05	181			
4.700E+05	182	36		
4.650E+05	183			
4.601E+05	184			
4.553E+05	185			
4.505E+05	186			
4.452E+05	187			
4.400E+05	188	37		
4.349E+05	189			
4.299E+05	190			
4.249E+05	191			
4.200E+05	192	38		
4.138E+05	193		11	
4.076E+05	194			
4.000E+05	195	39		11
3.938E+05	196			
3.877E+05	197			
3.829E+05	198			
3.782E+05	199			
3.735E+05	200			
3.688E+05	201			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
3.643E+05	202			
3.597E+05	203			
3.553E+05	204			
3.508E+05	205			
3.465E+05	206			
3.422E+05	207			
3.379E+05	208			
3.337E+05	209			
3.300E+05	210	40		
3.264E+05	211			
3.228E+05	212			
3.192E+05	213			
3.157E+05	214			
3.122E+05	215			
3.088E+05	216			
3.053E+05	217			
3.020E+05	218			
2.985E+05	219			
2.972E+05	220			
2.945E+05	221			
2.909E+05	222			
2.873E+05	223			
2.837E+05	224			
2.802E+05	225			
2.767E+05	226			
2.732E+05	227			
2.700E+05	228	41		
2.670E+05	229			
2.641E+05	230			
2.612E+05	231			
2.584E+05	232			
2.555E+05	233			
2.527E+05	234			
2.500E+05	235			
2.472E+05	236			
2.442E+05	237			
2.411E+05	238			
2.381E+05	239			
2.352E+05	240			
2.323E+05	241			
2.294E+05	242			
2.265E+05	243			
2.237E+05	244			
2.209E+05	245			
2.182E+05	246			
2.155E+05	247			
2.128E+05	248			
2.102E+05	249			
2.076E+05	250			
2.050E+05	251			
2.024E+05	252			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
2.000E+05	253	42		
1.962E+05	254			
1.926E+05	255			
1.902E+05	256			
1.878E+05	257			
1.855E+05	258			
1.832E+05	259			
1.809E+05	260			
1.786E+05	261			
1.764E+05	262			
1.742E+05	263			
1.721E+05	264			
1.699E+05	265			
1.678E+05	266			
1.657E+05	267			
1.637E+05	268			
1.616E+05	269			
1.596E+05	270			
1.576E+05	271			
1.557E+05	272			
1.538E+05	273			
1.519E+05	274			
1.500E+05	275	43		
1.481E+05	276			
1.463E+05	277			
1.445E+05	278			
1.426E+05	279			
1.409E+05	280			
1.391E+05	281			
1.374E+05	282			
1.357E+05	283			
1.340E+05	284			
1.323E+05	285			
1.307E+05	286			
1.291E+05	287			
1.283E+05	288	44		
1.269E+05	289		12	
1.255E+05	290			
1.241E+05	291			
1.228E+05	292			
1.213E+05	293			
1.197E+05	294			
1.183E+05	295			
1.168E+05	296			
1.153E+05	297			
1.139E+05	298			
1.125E+05	299			
1.111E+05	300			
1.096E+05	301			
1.082E+05	302			
1.068E+05	303			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
1.054E+05	304			
1.040E+05	305			
1.027E+05	306			
1.013E+05	307			
1.000E+05	308	45		12
9.804E+04	309			
9.652E+04	310			
9.502E+04	311			
9.355E+04	312			
9.210E+04	313			
9.067E+04	314			
8.926E+04	315			
8.788E+04	316			
8.652E+04	317			
8.500E+04	318	46		
8.374E+04	319			
8.250E+04	320			
8.200E+04	321	47		
8.074E+04	322			
7.950E+04	323			
7.835E+04	324			
7.722E+04	325			
7.610E+04	326			
7.500E+04	327	48		
7.399E+04	328			
7.300E+04	329	49		
7.200E+04	330			
7.081E+04	331			
6.965E+04	332			
6.851E+04	333			
6.738E+04	334			
6.641E+04	335			
6.545E+04	336			
6.451E+04	337			
6.358E+04	338			
6.267E+04	339			
6.177E+04	340			
6.088E+04	341			
6.000E+04	342	50		
5.912E+04	343			
5.826E+04	344			
5.740E+04	345			
5.656E+04	346			
5.551E+04	347			
5.448E+04	348			
5.347E+04	349			
5.248E+04	350			
5.200E+04	351	51		
5.099E+04	352			
5.000E+04	353	52		
4.905E+04	354			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
4.812E+04	355			
4.721E+04	356			
4.631E+04	357			
4.565E+04	358			
4.500E+04	359	53		
4.446E+04	360			
4.393E+04	361			
4.340E+04	362			
4.288E+04	363			
4.237E+04	364			
4.186E+04	365			
4.136E+04	366			
4.087E+04	367			
4.042E+04	368			
3.998E+04	369			
3.955E+04	370			
3.912E+04	371			
3.869E+04	372			
3.827E+04	373			
3.786E+04	374			
3.744E+04	375			
3.704E+04	376			
3.663E+04	377			
3.624E+04	378			
3.584E+04	379			
3.545E+04	380			
3.507E+04	381			
3.468E+04	382			
3.431E+04	383			
3.367E+04	384			
3.304E+04	385			
3.243E+04	386			
3.183E+04	387			
3.136E+04	388			
3.090E+04	389			
3.045E+04	390			
3.000E+04	391	54		
2.962E+04	392		13	
2.924E+04	393			
2.887E+04	394			
2.850E+04	395			
2.812E+04	396			
2.774E+04	397			
2.737E+04	398			
2.700E+04	399		14	
2.653E+04	400			
2.606E+04	401			
2.580E+04	402			
2.552E+04	403			
2.520E+04	404			
2.500E+04	405	55		13

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
2.479E+04	406		15	
2.450E+04	407			
2.418E+04	408			
2.388E+04	409			
2.358E+04	410			
2.314E+04	411			
2.271E+04	412			
2.229E+04	413			
2.188E+04	414			
2.139E+04	415			
2.092E+04	416			
2.045E+04	417			
2.000E+04	418			
1.965E+04	419			
1.931E+04	420			
1.900E+04	421			
1.870E+04	422			
1.841E+04	423			
1.812E+04	424			
1.783E+04	425			
1.755E+04	426			
1.727E+04	427			
1.700E+04	428	56		14
1.674E+04	429			
1.649E+04	430			
1.623E+04	431			
1.599E+04	432			
1.574E+04	433			
1.550E+04	434			
1.527E+04	435			
1.503E+04	436			
1.476E+04	437			
1.450E+04	438		16	
1.424E+04	439			
1.398E+04	440			
1.373E+04	441			
1.348E+04	442			
1.324E+04	443			
1.300E+04	444	57		15
1.266E+04	445			
1.234E+04	446			
1.202E+04	447			
1.171E+04	448			
1.142E+04	449			
1.114E+04	450			
1.086E+04	451			
1.060E+04	452			
1.031E+04	453			
1.003E+04	454			
9.763E+03	455			
9.500E+03	456	58		16

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
9.307E+03	457			
9.119E+03	458			
8.975E+03	459			
8.834E+03	460			
8.694E+03	461			
8.557E+03	462			
8.422E+03	463			
8.289E+03	464			
8.159E+03	465			
8.030E+03	466	59		
7.908E+03	467			
7.787E+03	468			
7.669E+03	469			
7.552E+03	470			
7.437E+03	471			
7.323E+03	472			
7.212E+03	473			
7.102E+03	474			
6.954E+03	475			
6.809E+03	476			
6.667E+03	477			
6.528E+03	478			
6.392E+03	479			
6.258E+03	480			
6.128E+03	481			
6.000E+03	482	60		
5.879E+03	483			
5.761E+03	484			
5.645E+03	485			
5.531E+03	486			
5.400E+03	487			
5.250E+03	488			
5.100E+03	489			
4.960E+03	490			
4.850E+03	491			
4.740E+03	492			
4.620E+03	493			
4.500E+03	494			
4.400E+03	495			
4.307E+03	496			
4.202E+03	497			
4.099E+03	498			
3.998E+03	499			
3.900E+03	500	61		
3.819E+03	501			
3.740E+03	502	62		
3.707E+03	503		17	
3.616E+03	504			
3.527E+03	505			
3.440E+03	506			
3.355E+03	507			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
3.272E+03	508			
3.191E+03	509			
3.112E+03	510			
3.035E+03	511			
3.000E+03	512	63	18	17
2.935E+03	513			
2.871E+03	514			
2.808E+03	515			
2.747E+03	516			
2.679E+03	517			
2.613E+03	518			
2.580E+03	519	64		18
2.532E+03	520		19	
2.485E+03	521			
2.435E+03	522			
2.386E+03	523			
2.337E+03	524			
2.290E+03	525	65		19
2.249E+03	526		20	
2.200E+03	527	66		20
2.158E+03	528		21	
2.116E+03	529			
2.075E+03	530			
2.035E+03	531			
2.004E+03	532			
1.973E+03	533			
1.943E+03	534			
1.914E+03	535			
1.885E+03	536			
1.856E+03	537			
1.828E+03	538			
1.800E+03	539	67		21
1.772E+03	540			
1.744E+03	541			
1.716E+03	542			
1.689E+03	543			
1.662E+03	544			
1.636E+03	545			
1.610E+03	546			
1.585E+03	547			
1.550E+03	548	68		
1.525E+03	549			
1.500E+03	550	69		
1.482E+03	551			
1.464E+03	552			
1.446E+03	553			
1.429E+03	554			
1.411E+03	555			
1.394E+03	556			
1.377E+03	557			
1.361E+03	558			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
1.344E+03	559			
1.328E+03	560		22	
1.312E+03	561			
1.296E+03	562			
1.280E+03	563			
1.265E+03	564			
1.249E+03	565			
1.234E+03	566			
1.213E+03	567			
1.191E+03	568			
1.171E+03	569			
1.150E+03	570	70		
1.137E+03	571			
1.125E+03	572			
1.112E+03	573			
1.100E+03	574			
1.087E+03	575			
1.075E+03	576			
1.063E+03	577			
1.051E+03	578			
1.040E+03	579			
1.028E+03	580			
1.017E+03	581			
1.005E+03	582			
9.940E+02	583			
9.829E+02	584			
9.720E+02	585			
9.611E+02	586			
9.555E+02	587			
9.500E+02	588	71		22
9.360E+02	589			
9.221E+02	590			
9.085E+02	591			
8.950E+02	592			
8.818E+02	593			
8.688E+02	594			
8.559E+02	595			
8.433E+02	596			
8.308E+02	597			
8.185E+02	598			
8.064E+02	599			
7.945E+02	600			
7.827E+02	601			
7.712E+02	602			
7.598E+02	603			
7.485E+02	604			
7.400E+02	605			
7.316E+02	606			
7.232E+02	607			
7.150E+02	608			
7.069E+02	609			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
6.988E+02	610			
6.909E+02	611			
6.830E+02	612	72		
6.765E+02	613			
6.700E+02	614	73		
6.585E+02	615		23	
6.471E+02	616			
6.359E+02	617			
6.250E+02	618			
6.142E+02	619			
6.036E+02	620			
5.932E+02	621			
5.830E+02	622			
5.745E+02	623			
5.662E+02	624			
5.581E+02	625			
5.500E+02	626	74		23
5.435E+02	627			
5.370E+02	628			
5.306E+02	629			
5.243E+02	630			
5.180E+02	631			
5.118E+02	632			
5.057E+02	633			
4.997E+02	634			
4.937E+02	635			
4.879E+02	636			
4.821E+02	637			
4.763E+02	638			
4.706E+02	639			
4.650E+02	640			
4.595E+02	641			
4.540E+02	642			
4.470E+02	643			
4.400E+02	644			
4.332E+02	645			
4.265E+02	646			
4.199E+02	647			
4.134E+02	648			
4.070E+02	649			
4.007E+02	650			
3.944E+02	651			
3.883E+02	652			
3.823E+02	653			
3.764E+02	654			
3.705E+02	655			
3.648E+02	656			
3.591E+02	657			
3.536E+02	658			
3.471E+02	659			
3.408E+02	660			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
3.345E+02	661			
3.284E+02	662			
3.224E+02	663			
3.165E+02	664			
3.107E+02	665			
3.050E+02	666	75		
2.999E+02	667			
2.948E+02	668			
2.899E+02	669			
2.850E+02	670	76		
2.801E+02	671		24	
2.754E+02	672			
2.707E+02	673			
2.661E+02	674			
2.615E+02	675			
2.571E+02	676			
2.527E+02	677			
2.484E+02	678			
2.442E+02	679			
2.400E+02	680	77		24
2.367E+02	681		25	
2.333E+02	682			
2.301E+02	683			
2.269E+02	684			
2.237E+02	685			
2.206E+02	686			
2.175E+02	687			
2.145E+02	688			
2.122E+02	689			
2.100E+02	690	78		25
2.088E+02	691		26	
2.075E+02	692	79		26
2.036E+02	693		27	
1.999E+02	694			
1.962E+02	695		28	
1.925E+02	696	80		27
1.892E+02	697			
1.860E+02	698	81		28
1.835E+02	699			
1.811E+02	700			
1.786E+02	701			
1.763E+02	702			
1.739E+02	703			
1.716E+02	704			
1.693E+02	705			
1.670E+02	706			
1.650E+02	707			
1.625E+02	708			
1.600E+02	709			
1.575E+02	710			
1.550E+02	711			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
1.525E+02	712			
1.500E+02	713			
1.475E+02	714			
1.450E+02	715			
1.425E+02	716			
1.400E+02	717			
1.375E+02	718			
1.350E+02	719			
1.325E+02	720			
1.301E+02	721			
1.280E+02	722			
1.260E+02	723			
1.240E+02	724			
1.220E+02	725	82		
1.205E+02	726		29	
1.190E+02	727	83		29
1.170E+02	728		30	
1.150E+02	729	84		30
1.130E+02	730			
1.105E+02	731			
1.080E+02	732	85		
1.063E+02	733		31	
1.038E+02	734			
1.013E+02	735			
1.000E+02	736	86		31
9.750E+01	737			
9.500E+01	738			
9.250E+01	739			
9.000E+01	740	87		
8.800E+01	741		32	
8.600E+01	742			
8.400E+01	743			
8.200E+01	744	88		32
8.100E+01	745		33	
8.000E+01	746	89		33
7.945E+01	747			
7.889E+01	748			
7.745E+01	749			
7.600E+01	750	90		
7.400E+01	751			
7.200E+01	752	91		
6.975E+01	753		34	
6.750E+01	754	92		34
6.625E+01	755		35	
6.500E+01	756	93	36	35
6.322E+01	757			
6.144E+01	758		37	
6.122E+01	759			
6.100E+01	760	94		36
6.000E+01	761			
5.900E+01	762	95		37

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
5.620E+01	763			
5.340E+01	764	96		
5.270E+01	765			
5.200E+01	766	97		
5.130E+01	767			
5.060E+01	768	98		
4.990E+01	769			
4.920E+01	770	99		
4.875E+01	771			
4.830E+01	772	100		
4.808E+01	773			
4.785E+01	774			
4.743E+01	775			
4.700E+01	776	101		
4.610E+01	777			
4.520E+01	778	102		
4.460E+01	779			
4.400E+01	780	103		
4.320E+01	781			
4.240E+01	782	104		
4.170E+01	783		38	
4.100E+01	784	105		38
4.030E+01	785		39	
3.960E+01	786	106		39
3.935E+01	787		40	
3.910E+01	788	107		40
3.855E+01	789		41	
3.800E+01	790	108		41
3.763E+01	791		42	
3.727E+01	792			
3.713E+01	793			
3.700E+01	794	109		42
3.625E+01	795		43	
3.550E+01	796	110		43
3.505E+01	797			
3.460E+01	798	111		
3.418E+01	799			
3.375E+01	800	112		
3.350E+01	801			
3.325E+01	802	113		
3.250E+01	803			
3.175E+01	804	114		44
3.150E+01	805			
3.125E+01	806	115		
3.063E+01	807		44	
3.000E+01	808	116		
2.951E+01	809			
2.902E+01	810			
2.826E+01	811			
2.750E+01	812	117		
2.625E+01	813			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
2.500E+01	814	118		
2.375E+01	815			
2.250E+01	816	119		
2.175E+01	817		45	
2.100E+01	818	120		45
2.050E+01	819		46	
2.000E+01	820	121		46
1.950E+01	821		47	
1.900E+01	822	122		
1.875E+01	823			
1.850E+01	824	123		47
1.805E+01	825			
1.760E+01	826			
1.730E+01	827			
1.700E+01	828	124		
1.650E+01	829			
1.600E+01	830	125		
1.555E+01	831			
1.510E+01	832	126		
1.475E+01	833			
1.440E+01	834	127		
1.408E+01	835			
1.375E+01	836	128		
1.333E+01	837		48	
1.290E+01	838	129		48
1.240E+01	839			
1.190E+01	840	130		
1.170E+01	841			
1.150E+01	842	131		
1.109E+01	843		49	
1.068E+01	844			
1.034E+01	845			
1.000E+01	846	132		49
9.550E+00	847			
9.100E+00	848	133		
8.708E+00	849			
8.315E+00	850			
8.208E+00	851			
8.100E+00	852	134		
7.625E+00	853			
7.150E+00	854	135		
7.075E+00	855		50	
7.000E+00	856	136		50
6.875E+00	857		51	
6.750E+00	858	137		51
6.625E+00	859		52	
6.500E+00	860	138		52
6.375E+00	861		53	
6.250E+00	862	139		53
6.000E+00	863	140		
5.850E+00	864			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
5.700E+00	865			
5.550E+00	866			
5.400E+00	867	141		
5.250E+00	868			
5.044E+00	869			
5.000E+00	870	142		54
4.875E+00	871		54	
4.750E+00	872	143		
4.500E+00	873			
4.300E+00	874			
4.150E+00	875			
4.000E+00	876	144		
3.928E+00	877			
3.830E+00	878			
3.730E+00	879	145		
3.620E+00	880			
3.500E+00	881	146		
3.300E+00	882			
3.150E+00	883	147		
3.050E+00	884	148		55
3.000E+00	885	149	55	
2.970E+00	886	150	56	56
2.920E+00	887		57	
2.870E+00	888	151		57
2.820E+00	889			
2.770E+00	890	152		
2.720E+00	891			
2.670E+00	892	153		
2.620E+00	893			
2.570E+00	894	154		
2.520E+00	895			
2.470E+00	896	155		
2.425E+00	897			
2.380E+00	898	156		
2.340E+00	899			
2.300E+00	900	157		
2.255E+00	901		58	
2.210E+00	902	158		58
2.165E+00	903			
2.120E+00	904	159		
2.060E+00	905			
2.000E+00	906	160		
1.970E+00	907			
1.940E+00	908	161		
1.900E+00	909			
1.860E+00	910	162		
1.815E+00	911			
1.770E+00	912	163		
1.725E+00	913			
1.680E+00	914	164		
1.635E+00	915			

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
1.590E+00	916	165		
1.545E+00	917		59	
1.500E+00	918	166		59
1.450E+00	919	167		
1.400E+00	920	168		
1.350E+00	921	169		
1.300E+00	922	170		
1.250E+00	923	171		
1.225E+00	924	172		
1.200E+00	925	173		60
1.175E+00	926	174	60	
1.150E+00	927	175		
1.140E+00	928	176		
1.130E+00	929	177		
1.120E+00	930	178		61
1.110E+00	931	179	61	
1.100E+00	932	180		
1.090E+00	933	181		
1.080E+00	934	182		
1.070E+00	935	183		
1.060E+00	936	184		
1.050E+00	937	185		
1.040E+00	938	186		
1.030E+00	939	187		
1.020E+00	940	188		
1.010E+00	941	189		
1.000E+00	942	190		
9.750E-01	943	191	62	62
9.500E-01	944	192		
9.250E-01	945	193		
9.000E-01	946	194		
8.764E-01	947			
8.500E-01	948	195		
8.000E-01	949	196		
7.500E-01	950	197		
7.000E-01	951	198		
6.826E-01	952			
6.500E-01	953	199		
6.250E-01	954	200	63	63
6.000E-01	955	201		
5.500E-01	956	202		
5.316E-01	957			
5.000E-01	958	203		
4.500E-01	959	204		
4.140E-01	960		64	
4.000E-01	961	205		64
3.750E-01	962	206	65	65
3.668E-01	963		66	
3.500E-01	964	207		66
3.250E-01	965	208	67	67
3.000E-01	966	209		

Upper neutron energy (eV)	999-group structure	SCALE 238-group structure	81A groups	81B3,C groups
2.750E-01	967	210	68	68
2.500E-01	968	211	69	69
2.250E-01	969	212	70	70
2.000E-01	970	213	71	71
1.840E-01	971			
1.750E-01	972	214		
1.500E-01	973	215	72	72
1.250E-01	974	216		
1.000E-01	975	217	73	73
9.000E-02	976	218		
8.000E-02	977	219		
7.000E-02	978	220	74	74
6.000E-02	979	221		
5.000E-02	980	222	75	75
4.000E-02	981	223	76	76
3.000E-02	982	224	77	77
2.530E-02	983	225	78	78
2.100E-02	984		79	
1.850E-02	985			
1.450E-02	986			
1.000E-02	987	226		79
7.500E-03	988	227	80	80
5.000E-03	989	228		
4.000E-03	990	229		
3.000E-03	991	230	81	81
2.500E-03	992	231		
2.000E-03	993	232		
1.500E-03	994	233		
1.200E-03	995	234		
1.000E-03	996	235		
7.500E-04	997	236		
5.000E-04	998	237		
1.000E-04	999	238		

3.3.2 Library 81B

Because the energy boundaries chosen for 81A did not always coincide with the energy boundaries used in SCALE's 238-group libraries, it was decided to make minor adjustments to the 81A-group structure so that it would align with the 238-group neutron energy group definitions. This alignment allows for easier comparisons between the broad-group and fine-group libraries. The 81B broad-group library (Table 3.1) was generated from the SCALE 238-group V7-238 library using a weighting function based on an HTGR 238-group neutron flux solution. The HTGR model used to calculate the neutron flux solution weighting function is listed in Appendix B. The 81B energy boundaries were selected to minimize differences with the 81A library energy boundaries.

3.3.3 Library 81B2

The broad-group library 81B2 used the same neutron energy group structure that was used in the generation of library 81B, but the library was generated using SCALE/MALOCS by condensing from the 999-group fine-group library using an appropriate 999-group HTGR neutron flux solution as the weighting function. This library should better represent the HTGR solution as it is based on the much finer detail of the SCALE 999-group master library and the ultra fine neutron flux solution in 999 groups.

3.3.4 Library 81B3

Broad-group library 81B3 was generated directly from ENDF/B-VII nuclear data files using an HTGR weighting function (flux solution) calculated with the CENTRM module in SCALE. The SCALE input case used to calculate the CENTRM flux weighting function is listed in Appendix C. The same neutron energy boundary structure was used with library 81B3 as with libraries 81B and 81B2.

Section 2.4 discusses the methodology employed in generating broad-group libraries directly from ENDF/B-VII nuclear data files. The SCALE input file listed in Appendix C was used to calculate the 1800K HTGR weighting function based on the CENTRM pointwise flux. This weighting approach is different from the method used in the generation of the generic 999-group fine-group library from the ENDF/B-VII files. The 999-group library was generated using the same weighting spectrum as all previous multigroup SCALE libraries, consisting of

1. Maxwellian spectrum (peak at 300 K) from 10−5 to 0.125 eV,
2. a 1/E spectrum from 0.125 eV to 67.4 keV,
3. a fission spectrum (effective temperature at 1.273 MeV) from 67.4 keV to 10 MeV, and
4. a 1/E spectrum from 10 to 20 MeV.

The use of a weighting function that is based on the CENTRM pointwise flux from a representative HTGR model simulation is a new technique developed at ORNL during this work. The temperature (1800K) considered in the calculation of the pointwise weighting function was considered appropriate for the high-temperature operation of an HTGR. This corresponds to a representative temperature of 1527°C, or 2780°F.

The initial version of this library (81B3i) created from the ENDF/B-VII data was then processed and enhanced with new IR f-factors and lambda factors for ^{238}U. The IR factors can be used with the new BONAMI-IR module to produce results that are generally equivalent to results with CENTRM/PMC, thus removing the need to run CENTRM/PMC for each unit cell. Thus, the IR capability can result in significant speedups in computer runtime compared with the traditional resonance self-shielding methods in SCALE.

3.3.5 Library 81C

The final broad-group nuclear data library, 81C, is based on the testing and improvements to library 81B3. This library is the ultimate result and includes new f-factors for ^{238}U and other actinides (App. F) and lambda factors for all nuclides. The neutron energy group boundaries are the same as the broad-group library 81B3. Broad-group library 81C, in addition to having all the necessary IR treatment factors implemented, also uses the new nuclide identification naming convention that has been developed to remove the maximum mixture number limit of 2147 in SCALE.

4. COMPARISON OF RESULTS WITH THE SCALE BROAD-GROUP LIBRARIES

Tables 4.1–4.3 summarize simplified model results with SCALE using various fine- and broad-group nuclear data libraries. The final 81C library is intended for use in production runs with SCALE. This broad-group library can model HTGR scenarios adequately, with similar accuracy to fine-group library runs but with considerably less computational time for resonance self-shielding of the cross sections. In the results presented in this section, BONAMI-IR and the 81C library ran 35 to 100 times faster than CENTRM/PMC with the same library.

Table 4.1 shows the results for a series of KENO MG cases for a homogenous HTGR pin cell model that is representative of a prismatic NGNP design. These results are compared with the 999 group library eigenvalue solution. The results obtained with the various 81-group libraries compare quite favorably with respect to the 238-group KENO result. The cases in Table 4.1 all use CENTRM cross-section processing with white boundary conditions at a temperature of 300K.

Table 4.1. k_{eff} comparisons for MG KENO homogeneous cell HTGR model

Libraries	k_{eff}	Δk relative to 999-group result (pcm)
81A	1.25766 ± 0.00039	-300 ± 81
81B	1.25746 ± 0.00040	-320 ± 83
81C	1.25586 ± 0.00040	-480 ± 82
238	1.25769 ±0.00041	-376 ± 88
999	1.26066 ± 0.00042	N/A

Table 4.2 shows results of a very simple XSDRN 1-D homogeneous HTGR core model at 300K and 1200K. Results using BONAMI-IR and the 81C Library are compared with cases using CENTRM with the 81C, 238-group, and 999-group libraries. Note that the CENTRM cases use a triangular pitch lattice cell that produces homogenized number densities for the 1-D XSDRN model. This simple model is not as precise as the benchmark cases that follow.

Table 4.2. k_{eff} comparisons for homogeneous 1-D radial model

k_{eff}	T(K)	CENTRM	Δk_{eff} (pcm)[a]	BONAMI-IR	Δk_{eff} (pcm)[a]
81C	300	1.25214	-378	1.24397	-1195
238	300	1.25434	-158	N/A	N/A
999	300	1.25592	–	N/A	N/A
81C	1200	1.11115	-364	1.10665	-814
238	1200	1.11279	-200	N/A	N/A
999	1200	1.11479	–	N/A	N/A

[a] Difference from CENTRM case with 999 groups at same temperature.

The High Temperature Engineering Test Reactor (HTTR) [12,13], which is the first HTGR in Japan, is a prismatic fuel graphite-moderated and helium-cooled reactor with a thermal output of 30 MW and a maximum outlet gas temperature of 950 °C and has the capability to demonstrate nuclear process heat utilization using an intermediate heat exchanger. The construction of the HTTR was decided by Japanese Atomic Energy Commission (JAEC) in 1987 and started in March 1991 by the Japan Atomic Energy Research Institute (JAERI) to establish and upgrade the technology basis for an HTGR. The HTTR was intended to serve as a potential tool for new and innovative basic research on high temperature technologies.

Calculations were performed in this work with two of the HTTR benchmark cases (case 1 and case 2) from the SCALE HTGR validation report [14]. The case 2 input file is listed in Appendix D, and both a cross-sectional and a vertical view of this HTTR model are shown in Appendix E. The calculated k_{eff} results,and the relative Δk values with respect to the CE KENO results are tabulated in Table 4.3 and 4.4. The results obtained with the 81C library and BONAMI-IR show good agreement with both the 238-group library and the CE results.

Table 4.3. k_{eff} results for HTTR benchmark case 1

Library	Cross-section processor	k_{eff}	Δk_{eff} (pcm) relative to CE
81C	BONAMI-IR	1.21629 ± 0.00024	-305 ± 49
81C	CENTRM	1.21661 ± 0.00022	-273 ±47
238	CENTRM	1.21887 ± 0.00025	-47 ± 50
999	CENTRM	1.21807 ± 0.00023	-127 ± 48
CE	N/A	1.21934 ± 0.00025	–

Table 4.4. k_{eff} results for HTTR benchmark case 2

Library	Cross-section processor	k_{eff}	Δk_{eff} (pcm) relative to CE
81C	BONAMI-IR	1.20799 ± 0.00027	-374 ± 52
81C	CENTRM	1.20659 ± 0.00029	-514 ± 54
238	CENTRM	1.20930 ± 0.00023	-243 ± 48
CE	N/A	1.21173 ± 0.00025	–

The performance of the 81C library for analyses of pebble bed reactor (PBR) configurations was assessed using two test cases: (1) a pebble unit cell with fuel representative of the HTR-10 reactor at full power and (2) the first critical core of HTR-10. The models that were used for testing are described in detail elsewhere [14]. The model for the pebble unit cell is a 1-D SCALE/XSDRN model. The model for the first critical core of HTR-10 is a full 3-D SCALE/KENO-VI model that has been developed using benchmark specifications included in the IRPhE Handbook [15]. The double heterogeneity of fuel is modeled in SCALE using the DOUBLEHET option for multigroup cross-section processing.

The results obtained with SCALE for the pebble unit cell at operating temperature (1200K for fuel and 900K for coolant) are presented in Table 4.5, as obtained using the 81C HTGR library and the standard 238-group ENDF/B-VII transport library in SCALE. The 81C library was used with both CENTRM and the new BONAMI-IR for cross section self-shielding. Also shown in Table 4.5 is the result obtained with MCNP5 continuous energy ENDF/B-VII data for the same configuration. The MCNP5 model explicitly

represents the fuel particles inside the fuel pebbles using a lattice representation that ensures the fuel particles do not intersect the interface of the graphite matrix with the pebble shell [14]. The result obtained with the 81-group library and BONAMI-IR is within 146 pcm of the SCALE result for the 238-group library and within 271 pcm of the MCNP result.

Table 4.5. k_{eff} results for HTR-10 pebble unit cell (1200K fuel, 900K coolant)

Code	Library	Cross-section processor	k_{eff}	Δk_{eff} (pcm)[d]	Δk_{eff} (pcm)[e]
MCNP	CE[a] ENDF/B-VII	NA[b]	1.60822 (σ=0.00021)[c]	–	-125
SCALE	238-group ENDF/B-VII	CENTRM	1.60936	125	–
	81C	CENTRM	1.60783	-28	-153
	81C	BONAMI-IR	1.61082	-271	146

[a] CE = continuous energy.
[b] NA = not applicable.
[c] Standard deviation from the Monte Carlo transport calculation.
[d] Difference in k_{eff} is calculated using the MCNP result as reference; 1 pcm=10^{-5}.
[e] Difference in k_{eff} is calculated using the SCALE 238-group ENDF/B-VII with CENTRM result as reference.

To assess the effect of the temperature on library performance, the same pebble unit cell was calculated with 300K temperature in both fuel and coolant. The corresponding results are presented in Table 4.6. If the SCALE result for the 238-group library is used as the reference for comparison, the result obtained with the 81-group library is within 148 pcm when using CENTRM and within 338 pcm when using BONAMI-IR.

Table 4 6. k_{eff} results for HTR-10 pebble unit (300K)

Code	Library	Cross-section Processor	k_{eff}	Δk_{eff} (pcm)[d]	Δk_{eff} (pcm)[e]
MCNP	CE[a] ENDF/B-VII	NA[b]	1.69040 (σ=0.00014)[c]	–	110
SCALE	238-group ENDF/B-VII	CENTRM	1.68930	-110	–
	81C	CENTRM	1.68782	-258	-148
	81C	BONAMI-IR	1.68592	-448	-338

[a] CE = continuous energy.
[b] NA = not applicable.
[c] Standard deviation from the Monte Carlo transport calculation.
[d] Difference in k_{eff} is calculated using the MCNP result as reference; 1 pcm=10^{-5}.
[e] Difference in k_{eff} is calculated using the SCALE 238-group ENDF/B-VII with CENTRM result as reference.

The results obtained for the HTR-10 first core (full core 3-D model) are shown in Table 4.7. There is an excellent agreement between MCNP and SCALE when using the 238-group ENDF/B-VII library. The result obtained with the 81-group library and BONAMI-IR is within 357 pcm of the 238-group library result with CENTRM. This difference is consistent with the difference seen in Table 4.6 for the pebble unit cell at the same temperature (300 K).

Table 4.7. k_{eff} results for HTR-10 full core

Code	Library	Cross-section processor	k_{eff}	Δk_{eff} (pcm)[d]	Δk_{eff} (pcm)[c]
MCNP	CE[a] ENDF/B-VII	NA[b]	1.01473 (σ=0.00021)[c]	–	54 ± 85
SCALE	238-group ENDF/B-VII	CENTRM	1.01419 (σ=0.00082)	-54 ± 85	–
	81C	BONAMI-IR	1.01062 (σ=0.00087)	-411 ± 89	-357 ± 120

[a] CE = continuous energy.
[b] NA = not applicable.
[c] Standard deviation from the Monte Carlo transport calculation.
[d] Difference in k_{eff} is calculated using the MCNP result as reference; 1 pcm=10^{-5}.
[e] Difference in k_{eff} is calculated using the SCALE 238-group ENDF/B-VII with CENTRM result as reference.

The calculated results with BONAMI-IR and the 81C library for the HTTR and HTR-10 reactor benchmarks demonstrate the capability to produce accurate results for actual operating HTGRs, both with prismatic and pebble bed fuels. These results show good agreement with CE and 238-group calculations. Although further verification and validation of BONAMI-IR and the 81C library are desirable, these results presented here provide confidence that this library can be useful for HTGR analyses.

5. SUMMARY AND RECOMMENDATIONS

The final 81-group library allows for the modeling of HTGR cases with SCALE with sufficient accuracy and faster CPU times than the V7-238 library. Further processing to include intermediate resonance features provides an additional improvement by reducing computational times for resonance self-shielding (up to 100 times faster) without loss of accuracy.

We observed that

1. HTGR broad-group libraries need more groups than LWR broad-group libraries.
2. In HTGRs, the average neutron flux distribution in the vicinity of fuel is more important for neutronics and self-shielding considerations than the flux within the fuel.
3. Fine-group libraries with many groups (such as the new 999-group library) properly show details of the increase in flux at the lower end of resonances, due to the self-shielding of the resonance and the reduction in cross section at the lower energy.
4. The use of flux values from the average flux distribution of an HTGR model is an appropriate weighting function for use in the generation of broad-group libraries.

The effectiveness and correctness of a broad-group nuclear data library is quite sensitive to the neutron energy boundary structure and to the weighting function (usually a fine-group neutron flux solution) that is used in generating the library from ENDF/B files or through condensation from a fine-group master library.

Based on the results presented in this report, the choice of the broad-group energy boundaries for 81C library allows SCALE to model HTGR cases with reasonable accuracy and significantly faster CPU times than fine-group or CE calculations. The new 81C library includes new lambda factors for all nuclides and f-factors for ^{238}U and other actinides. It also contains high-temperature data consistent with HTGR operation and modeling. The 81C library requires the BONAMI-IR module in SCALE to fully utilize data in the library. When the IR data are processed with BONAMI-IR, accurate results can be obtained with significantly reduced computational runtimes.

6. REFERENCES

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APPENDIX A

DESCRIPTION OF INTERMEDIATE RESONANCE METHOD IN SCALE

A.1 INTERMEDIATE RESONANCE APPROXIMATION

The intermediate resonance (IR) approximation was proposed in the 1960s as an extension to the narrow resonance (NR) and wide resonance (WR) approximations, which are used in solving the slowing-down equation to obtain an analytical flux expression for computing multigroup (MG) cross sections. The NR approximation is used to represent elastic scattering sources of nuclides for which the neutron energy loss is large compared to the practical width of resonances for the absorber materials of interest. This approximation tends to be more accurate for light nuclides (e.g., moderators) and for higher energy ranges. Conversely, the WR approximation is used to represent elastic scattering sources of nuclides for which the neutron energy loss is small compared to the practical widths. This approximation tends to be more accurate for heavy nuclides (e.g., the limit of infinite mass is usually assumed) and for lower energy ranges. Since most resonance absorption in LEU thermal reactors occurs in ^{238}U, this material is usually used as the basis to determine if a nuclide is a NR or a WR scatterer.

Many materials cannot be treated accurately by either the NR or WR methods. The IR method provides a more generalized approach in which the scattering source is represented by a linear combination of NR and WR expressions; i.e., for scatterers with slowing-down properties intermediate between NR and WR scatterers. This is done by introducing an IR parameter usually called lambda factors, for which NR scatters have λ=1, WR scatters have λ=0, and fractional λ's are for intermediate scatterers. Codes have been developed by ORNL to determine group-dependent lambda values for all materials, using the procedure described in Section A.2. Lambda values are included in the HTR 81-group library.

Applying the IR approximation and neglecting resonance overlap effects in the slowing-down equation, the following analytical expression is obtained for the flux spectrum near a resonance of nuclide "r":

$$\Phi_{IR}^{(r)}(E;\sigma_0^{(r)}) = \left(\frac{\sigma_p^{(r)}+\sigma_0^{(r)}}{\sigma_t^{(r)}(E)+\sigma_0^{(r)}}\right)\frac{1}{E}$$

where $\sigma_t^{(r)}(E)$, $\sigma_p^{(r)}$, $\sigma_0^{(r)}$ are the total, potential, and background cross sections for resonance material "r".

The background cross section in Eq. 1 depends on the lambda factors and is equal to

$$\sigma_0^{(r)} = \frac{1}{N^{(r)}}\sum_{j\neq r}\lambda^{(j)}\Sigma_p^{(j)}$$

Equation 2 is appropriate for a homogeneous medium, but a similar expression also can be used for heterogeneous lattices by including an additional constant called the escape cross section. Eq. 1 shows that the IR method allows the flux energy spectrum to be parameterized in terms of the single variable $\sigma_0^{(r)}$, which indicates the degree of resonance self-shielding. The value of $\sigma_0^{(r)}$ can vary by multigroup, but it is not a function of energy within a group.

Energy-dependent spectra for weighting MG cross sections of an arbitrary resonance material "r" are obtained by solving the slowing-down equation with the pointwise code CENTRM for a homogeneous mixture composed of "r" plus hydrogen. The hydrogen concentration is varied to produce the desired background cross sections in a predetermined set that spans the expected range of self-shielding for the resonance material, so that a set of MG data are computed at varying degrees of self-shielding. These are

converted into group-dependent self-shielding factors parameterized versus $\sigma_0^{(r)}$, which are stored on the AMPX master library.

During a reactor physics calculation with TRITON, for example, the background for the system of interest is computed using eq. 2 with problem-specific materials and concentrations, and the corresponding shielding factor is found by interpolating from the set of background cross sections on the library. This is done by the SCALE code BONAMI, which has been modified to use the IR expression for the background cross section. The self-shielded cross section for the particular system is equal to the product of the interpolated shielding factor and the unshielded (i.e., infinitely dilute) cross section, which is also stored in the master library. The BONAMI IR procedure for computing self-shielded cross sections is very fast since only data interpolation is required.

A.2 COMPUTATION OF HYDROGEN-EQUIVALENT LAMBDA FACTORS

An important component of the IR method is to have reasonable values for the IR lambda values. ORNL computes these values using the "hydrogen equivalence" approach based on ^{238}U resonances. In this well-established method, it is assumed that hydrogen is a true NR material (λ=1) since a neutron can lose essentially all of its energy in single elastic collision. A table of self-shielded cross sections versus background cross sections is generated for mixtures of ^{238}U and hydrogen with varying concentrations, using CENTRM calculations as described in the previous section. To obtain lambdas for nuclides other than hydrogen, a portion of the hydrogen number density in the mixture is replaced by another nuclide "*j*". If a one-to-one exchange of hydrogen atoms with atoms of "*j*" is done (i.e., number of hydrogen atoms removed equals the number of *j* added), the shielded cross section for the mixture will be different than the corresponding mixture containing only hydrogen, since the slowing-down properties of *j* are different. However instead of one-to-one replacement, the number of *j* atoms is modified to obtain the same shielded cross section as obtained with hydrogen. This is called the hydrogen equivalent number density of *j*, and from this value the corresponding lambda value for nuclide *j* can be found. The procedure is repeated for each multigroup to obtain group-dependent lambdas. The lambda factors are not very sensitive to temperature and thus have been generated only for the nominal fuel temperature of 1500 K in the HTR 81-group library.

APPENDIX B

INPUT FILE FOR RADIAL CORE MODEL 999-GROUP (VHTR) MODEL

Presented here is an input file for the radial_core_model-999grps (VHTR) model.

```
=shell
cp ~xxx/SCALE6/HTR_multigroup_proj/older_csas_decks/v7_999 v7_999
end
=csas1x          parm=centrm
homog (no double het) fuel unit cell for ngnp prismatic lattice
v7_999
read comp
'
'
'    This case does not collapse to 23-Groups
'
'
'
'
' homgenized channel
u-238     1 0 7.99688E-4 300.0 end
u-235     1 0 7.23460E-5 300.0 end
o         1 0 1.30805E-3 300.0 end
graphite  1 0 5.85220e-2 300.0 end
graphite  1 0 3.77085E-3 300.0 end
si        1 0 3.77085E-3 300.0 end
'
' graphite moderator
graphite   7 den=1.74 1.0  300.0 end
'
' helium coolant
he-3      8 0 3.71220e-11 300.0 end
he-4      8 0 2.65156e-5 300.0 end
'
' carbon steel for PV
carbonsteel 91  end
'
' S.S. for structure
ss316       92  end
'
' graphite reflector
graphite    93 den=1.74 1.0  300.0 end
b-11        93 0  1.0e-8 300.0  end
b-10        93 0  0.2e-8 300.0  end
'
end comp
read celldata
  lattice triangpitch pitch=1.8796 7 fuelr=0.6225 1
  gapr=0.6350 8 cellmix=40  end
  centrm data
    ixprt=1 ipbt=1
'   reflected BC in CENTRM
    ibr=1  iup=20 demin=2.0E-5
  end centrm
end celldata
end
=shell
rm ft02f001
```

```
rm ft03f001
rm ft42f001
rm ft81f001
end
=xsdrn
Radial model of VHTR, with homo 999 grp XSs (no double het).
' this case collapses over 3 zones: inner refl, core, and outer refl
'
'   ige izm  im ibl ibr  mx  ms  sn isct ievt iim  icm iclc ith
'1$$  2   3  334  1   0   2   11  8   3    1   20   60   30  0  e
1$$  2   3  334  1   0   2   11  8   3    1   20   600   500  0  e
'
'    iprt  id1  ipbt isx isen  idm2  nbands ifsn
'2$$  -2    -1    1    1   0     0     -2    0    e
2$$  -2    -1    1    1   0     0     -4    0    e
'
'    ifg  iqm  ipm  ifn  itmx  idat1  ipn  idfm  iaz  iai  ifct
'3$$   1    0    0    1    0      0     3    0     4    1    1   e
3$$   0    0    0    1    0      0     3    0     4    1    1   e
'
'    icon  igmf  itp  ipp
4$$   0     999    0     0      e
'
'     eps     ptc    xnf   ev evm bf     dy
'5**  1.0e-4  1.0e-5  1.0              a7 813.0  e
5**  1.0e-4  1.0e-6  1.0             a7 813.0  e
 T
'
'           <<   M I X I N G   T A B L E   >>
'
'   mixtures:  mix-1=homo fuel block  ;  mix-2=graphite reflector
13$$  10r1  2
'
'   nuclide iDs for cell-homogenized fuel XS ; reflector
14$$  1092238 1092235 1008016 1006312 1014028 1014029
      1014030 7006312 8002003 8002004     93006312
'
'  homo fuel atom densities ; and reflector
15**  3.18E-04 2.88E-05  1.093E-02 2.48E-02 1.38E-03 7.01E-05
      4.65E-05 5.12E-02 5.99E-13 4.28E-07   8.73211E-02
 T
'
' fission density guess
34##  f1.0
 T
' radial intervals
35**  146i0.0  32i147.62 32i180.31 27i213.01 92i241.32 334.40
'
' zone numbers by interval
'      -inner refl-    --  3 fuel rings  --    -- outer refl --
'      ------------    --------------------    ----------------
36$$   144r1  1 1 1    2 2 2  88r2  2 2 2         3 3 3   90r3
'
' mixture by zone
39$$  2  1  2
'
'  transport method by group, for iclc outers
```

```
46$$  148r0  f1
'
' activity materials
49$$  1092238  1092235  1092235 93006312
'
' activity mts
50$$  -102  -18  1452  -2
'
' was: collapsed group structure. set to 23 groups
'      51$$  11r1 6r2 17r3 10r4 5r5 8r6 17r7 69r8 22r9 14r10 5r11 6r12
'      4r13 8r14 2r15 2r16 2r17 2r18 3r19 1r20 2r21 5r22 17r23
'51$$ 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
'25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
'48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70
'71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93
'94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112
'113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129
'130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146
'147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163
'164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180
'181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197
'198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214
'215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231
'232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248
'249 250 251 252 253 254 255 256 257 258 259 260 261
T
end
'=shell
'rm ft04f001
'mv ft03f001 ft04f001
'end
=xsdrn
Radial model of VHTR, with full 999 grp XSs (no double het).
' uses 999-grp XSs collapsed over 3 zones (innr refl,core,outr refl)
'
'   ige izm  im ibl ibr  mx  ms  sn isct ievt iim  icm iclc ith
1$$  2   3  334  1   0   3   12  8   3    1   20   300  200    0  e
'
'    iprt  id1  ipbt isx isen  idm2  nbands ifsn
2$$  -2     0    0    0   0     0      -3    0    e
'
'    ifg  iqm  ipm  ifn  itmx  idat1  ipn  idfm  iaz  iai  ifct
3$$   0    0    0    1    0      0     3    0     4    1    1   e
'
'     eps     ptc    xnf   ev evm bf     dy
5**  1.0e-4  1.0e-6  1.0             a7 813.0  e
 T
'
'          <<   M I X I N G   T A B L E   >>
'
'   mixtures:  mix-1=homo fuel block  ;  mix-2=graphite reflector
13$$  10r1  2  3
'
'   nuclide iDs for cell-homogenized fuel XS ; reflector
14$$  21092238 21092235 21008016 21006312 21014028 21014029
      21014030 27006312 28002003 28002004  193006312  393006312
'
```

```
'  homo fuel atom densities ; and reflector
15**  3.18E-04 2.88E-05  1.093E-02 2.48E-02 1.38E-03 7.01E-05
     4.65E-05 5.12E-02 5.99E-13 4.28E-07   8.73211E-02  8.73211E-02
 T
'
' fission density guess
34##  f1.0
 T
' radial intervals
35**  146i0.0  32i147.62 32i180.31 27i213.01 92i241.32 334.40
'
' zone numbers by interval
'      -inner refl-    --  3 fuel rings  --    -- outer refl --
'      ------------    --------------------    ----------------
36$$   144r1  1 1 1    2 2 2  88r2  2 2 2         3 3 3   90r3
'
' mixture by zone
39$$  2  1  3
'
'  transport method by group, for iclc outers
46$$  8r0  f1
'
' activity materials
49$$  21092238  21092235  21092235 193006312
'
' activity mts
50$$  -102  -18  1452  -2
'
  T
end
```

APPENDIX C

INPUT FOR GENERATING CENTRM POINTWISE FLUX WEIGHTING FUNCTIONS

Presented here is an input file for generating a temperature-dependent CENTRM pointwise flux weighting function (this example for 1800 K).

```
=csas1x          parm=centrm
homo (NO double-het) fuel unit cell for ngp prismatic lattice
V7-238
read comp
' homgenized channel
u-238    1 0 7.99688E-4 1800.0 end
u-235    1 0 7.23460E-5 1800.0 end
o        1 0 1.30805E-3 1800.0 end
graphite 1 0 5.85220e-2 1800.0 end
' c        1 0 3.77085E-3 1800.0 end
graphite 1 0 3.77085E-3 1800.0 end
si       1 0 3.77085E-3 1800.0 end
'
' graphite moderator
graphite  7 den=1.74 1.0  300.0 end
'
' helium coolant
he-3      8 0 3.71220e-11 300.0 end
he-4      8 0 2.65156e-5 300.0 end
end comp
read celldata
lattice triangpitch pitch=1.5 7 fuelr=0.6225 1
    gapr=0.6350 8 end
centrm data ixprt=1 ipbt=1 nprt=1 iprt=-1 id1=2
' reflected BC in CENTRM
 isn=10
 n2d=0
 ibr=3
 iup=20
demin=2.0E-5
end centrm
moredata  szf=0.5  end
end celldata
end
```

APPENDIX D

INPUT FOR TEST2R3_MG: SAMPLE JAPANESE HTTR BENCHMARK CASE

Presented here is input for the Test2r3_Mg: sample Japanese HTTR benchmark case

```
=shell
cp /home/xxx/newlib_htgr/81B3/tst8_IR_Master ft34f001
ln -sf /home/xxx/SCALE6_100204/Linux_x86_64/bin/csas6 ./csas6
ln -sf /home/xxx/SCALE6_100204/Linux_x86_64/bin/bonami ./bonami
end
=ajax
0$$ 88 e
1$$ 1 t
2$$ 34 0 t
end
=csas26 parm=bonami
Volkan's test# 1: 5 rings of 6.3% enriched fuel blocks + 1 reflector ring
ft88f001
' ------------------------------------------------------------------------------
' --- References:
' [1] John D. Bess, Nozomu Fujimoto: Evaluation of the Start-up Core Physics Tests
'     at Japan's High Temperature Engineering Test Reactor (Fully-Loaded Core),
'     Revision 0, March, 2009

' ------------------------------------------------------------------------------
' --- Materials --------------------------------------------------------------
read comp
' Material References:
' --------------------
' m=7         CFP fuel atom densities from Table 3.1, pag. 195 of [1]
' m=13        Buffer atom densities from Table 3.2, pag. 196 of [1]
' m=14        IPyC atom densities from Table 3.2, pag. 196 of [1]
' m=15        SiC atom densities from Table 3.2, pag. 196 of [1]
' m=16        OPyC atom densities from Table 3.2, pag. 196 of [1]
' m=17        Overcoat atom densities from Table 3.2, pag. 196 of [1]
' m=18        Compact atom densities from Table 3.3, pag. 196 of [1]
' m=19        Sleeve atom densities from Table 3.4, pag. 196 of [1]
' m=20        IG-110 atom densities from Table 3.6, pag. 197 of [1]
'             by multiplying with 1.005
' m=21        Helium coolant from 3.1.3.10, page 199 of [1]
' m=22        Disks atom densities in BP pins from Table 3.5, pag. 197 of [1]
' m=24        BP atom densities (2.5%) from Table 3.5, pag. 197 of [1]
' m=25        PGX Graphite from Table 3.9, pag. 199 of [1]
'
' ==============================================================================
' --- Fuel Kernel, 6.3% enrichment:
  U-234           7  0   1.1293E-05   300.00  end
  U-235           7  0   1.4783E-03   300.00  end
  U-238           7  0   2.1699E-02   300.00  end
  O-16            7  0   4.6343E-02   300.00  end
  B-10            7  0   1.7276E-07   300.00  end
' --- Buffer:
  C-graphite     13  0   5.5153E-02   300.00  end
  B-10           13  0   1.8290E-08   300.00  end
' --- IPyC:
  C-graphite     14  0   9.2758E-02   300.00  end
  B-10           14  0   3.0761E-08   300.00  end
' --- SiC:
  C-graphite     15  0   4.8061E-02   300.00  end
  Si             15  0   4.8061E-02   300.00  end
  B-10           15  0   5.3208E-08   300.00  end
' --- OPyC:
  C-graphite     16  0   9.2758E-02   300.00  end
  B-10           16  0   3.0761E-08   300.00  end
' --- Graphite overcoat:
  C-graphite     17  0   8.5237E-02   300.00  end
```

```
  B-10           17  0   2.8267E-08   300.00  end
' --- Graphite compact:
  C-graphite     18  0   8.5237E-02   300.00  end
  B-10           18  0   1.5452E-08   300.00  end
' --- Graphite sleeve:
  C-graphite     19  0   8.8747E-02   300.00  end
  B-10           19  0   7.2596E-09   300.00  end
' --- IG-110 Graphite:
  C-graphite     20  0   8.8243E-02   300.00  end
  B-10           20  0   7.8036E-09   300.00  end
' --- Helium coolant:
  He             21  0   2.4616E-05   300.00  end
' --- Graphite disks:
  C-graphite     22  0   8.8747E-02   300.00  end
  B-10           22  0   7.2596E-09   300.00  end
' --- Burnable poison (2.5wt%):
  C-graphite     24  0   8.7995E-02   300.00  end
  B-10           24  0   4.9882E-04   300.00  end
  B-11           24  0   2.0078E-03   300.00  end
' --- PGX Graphite:
  C-graphite     25  0   8.6134E-02   300.00  end
  B-10           25  0   3.6372E-08   300.00  end
' --- Homogenized graphite compact (inner and outer helium embeded):
' Obtained by volumetric homogenization of materials 18 and 21
  He             28  0   4.6313E-06   300.00  end
  C-graphite     28  0   6.8834E-02   300.00  end
  B-10           28  0   4.7270E-09   300.00  end
end comp

' ------------------------------------------------------------------------
' --- Cell data ----------------------------------------------------------
read celldata
 doublehet fuelmix=10 end
    gfd=0.06       7
  coatr=0.036     13
  coatr=0.039     14
  coatr=0.0415    15
  coatr=0.046     16
 matrix=28
 numpar=12987 end grain
 rod triangpitch right_bdy=white left_bdy=reflected
 pitch=5.15 20 fuelr=1.3 fuelh=3.9 gapd=3.4 19 cladd=4.1 21 end
moredata iropt=1 end
end celldata

' ------------------------------------------------------------------------
' --- Parameters ---------------------------------------------------------
read parm
       gen=110
       npg=100000
       nsk=10
       tba=100
       htm=no
       flx=yes
       fdn=yes
end parm

' ------------------------------------------------------------------------
' --- Geometry -----------------------------------------------------------
read geom
' Dimensions for block and pin details based on Figure 1.52 page 68 of [1]
' Counting of pins starts at the lower left corner, going horizontally and
' then vertically
```

```
' Dimensions for grain cells based on Figure 3.1 page 176 of [1]
'
' Numbering scheme for cells that make up fuel block units:
'  zlb1   fuel grain
'  zlb2   BP pin
'  zlb3   fuel pin
'  zlb4   central hole
'  zlb5   empty pin
'  zlb6   graphite
'  zlb    block
'
' Block numbering (Fig. 3.15, page 190 of [1]):
' Each block is numbered according to the scheme 100*z+10*l+b, where:
'   z=1,...,8       zone number
'                      **Fuel: z=1,2 for zones 1 and 2, respectively
'                              z=3,5 alternatively as one goes counterclockwise
'                              for zone 3, z=4 for zone 4
'                      **Replaceable Reflectors in fuel columns follow the same
'                        pattern as fuel blocks, but with different l: l=1,2,8,9
'                      **CR:   z=6 for "C" (b=1) and "R1" (b=2,...,7)
'                              z=7 for "R2" and "R3" (b=1,...,9, going
'                              counterclockwise)
'                      **Instrumentation Blocks have z=8 (b=1,2,3)
'   l=1,...,9       layer number from top to bottom
'                   (fuel blocks in layers 3 to 7 from top)
'   b=1,...,bmax(z) block number (starting from pozitive x, counterclockwise)
'                      bmax(1)=...=bmax(5)=6
'                      bmax(6)=7, bmax(7)=9
'                      bmax(8)=3
' Replaceable Reflector (RR) blocks that are not in fuel columns are assigned
' block# 900
' Graphite blocks to make up the Permanent Reflector are assigned block# 100
'
'================ Graphite Block =================
unit 10
  hexprism      1  18.     29.    -29.
  media      25     1       1
  boundary      1
'================ Void Block =================
unit 20
  hexprism      1  18.     29.    -29.
  media       0     1       1
  boundary      1
'================ Central handling hole =================
unit 1114
  cone          1   2.5    29.      1.5    20.
  cylinder      2   1.5    20.     14.
  cylinder      3   2.25   14.      4.
  cylinder      4   2.505  29.    -29.
  hexprism      5   2.575  29.    -29.
  media      21     1       1
  media      21     1       2
  media      21     1       3
  media      20     1       4      -1      -2      -3
  media      20     1       5      -4
  boundary      5
'================ Graphite =================
unit 1116
  hexprism      1   2.575  29.    -29.
  media      20     1       1
  boundary      1
'================ Empty BP pin location =================
unit 1315
```

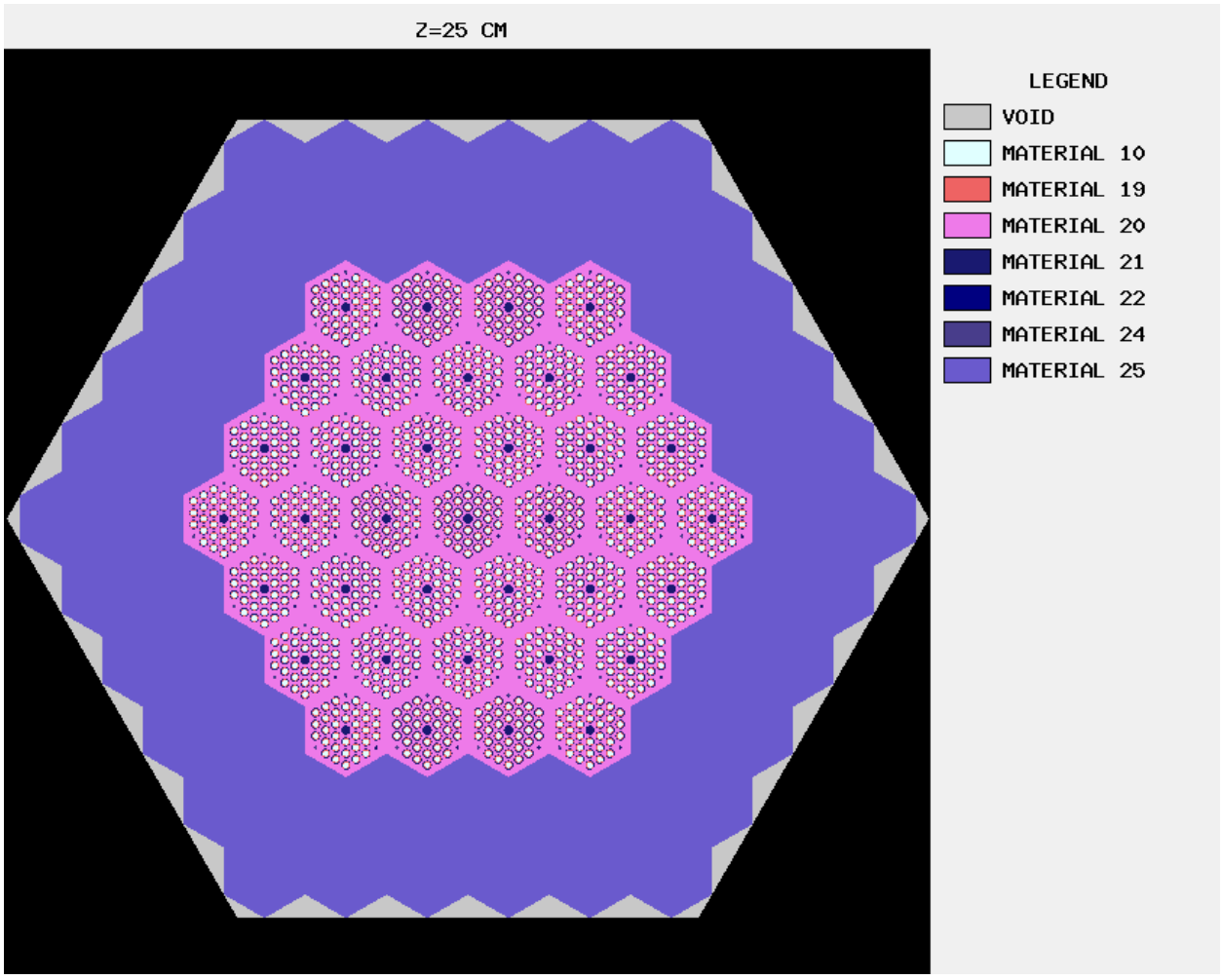
```
  cylinder      1   0.75   25.2   -24.8
  cylinder      2   0.75   29.    -29.
  hexprism      3   2.575  29.    -29.
  media      21     1       1
  media      20     1       2      -1
  media      20     1       3      -2
  boundary      3
'================ 2.5 wt% BP pin =================
unit 1412
  cylinder      1   0.7     5.2    -4.8
  cylinder      2   0.7    25.2   -24.8
  cylinder      3   0.75   25.2   -24.8
  cylinder      4   0.75   29.    -29.
  hexprism      5   2.575  29.    -29.
  media      22     1       1
  media      24     1       2      -1
  media      21     1       3      -2
  media      20     1       4      -3
  media      20     1       5      -4
  boundary      5
'================ Block 241 =================
unit 2413
  cylinder      2   1.3    27.3   -27.3
  cylinder      4   1.7    28.85  -28.85
  cylinder      5   2.05   29.    -29.
  hexprism      6   2.575  29.    -29.
  media      10     1       2
  media      19     1       4      -2
  media      21     1       5      -4
  media      20     1       6      -5
  boundary      6
unit 110
  rhexprism     1  17.     29.    -29.
  array  241  1  place  5  5  1   0.0      0.0      0.0
  boundary      1
unit 11
  hexprism      1  18.     29.    -29.
  hole  110  rotate a1=30
  media      20     1       1
  boundary      1
'================ Global Geometry =================
global unit 1
  rhexprism     1 176.669182      29.    -29.
  array    1  1  place   7   7  1   0.0      0.0      0.0
  boundary      1
end geom

' ------------------------------------------------------------------------------
' --- Boundary conditions ------------------------------------------------------
read boun
 surface(1)=vacuum
 surface(2)=vacuum
 surface(3)=vacuum
 surface(4)=vacuum
 surface(5)=vacuum
 surface(6)=vacuum
 surface(7)=reflect
 surface(8)=reflect
end boun

' ------------------------------------------------------------------------------
read array
  ara=1 nux=13 nuy=13 nuz=1 typ=hexagonal
```

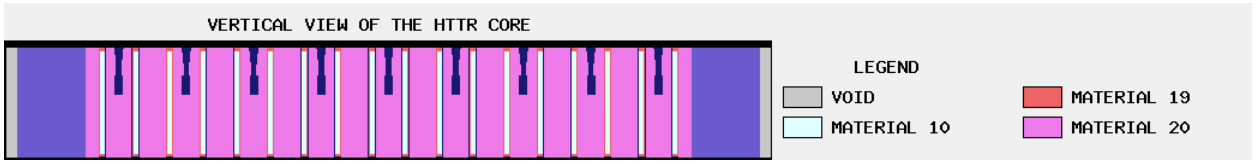
```
  fill
  20  20  20  20  20  20  20  20  20  20  20  20  20
    20  20  20  20  20  20  10  10  10  10  10  10  20
      20  20  20  20  20  10  10  10  10  10  10  10  20
        20  20  20  20  20  10  10  11  11  11  10  10  20
          20  20  20  10  10  11  11  11  11  11  10  10  20
            20  20  10  10  11  11  11  11  11  11  10  10  20
              20  10  10  11  11  11  11  11  11  11  10  10  20
                20  10  10  11  11  11  11  11  11  10  10  20  20
                  20  10  10  11  11  11  11  11  10  10  20  20  20
                    20  10  10  11  11  11  11  10  10  20  20  20  20
                      20  10  10  10  10  10  10  10  20  20  20  20  20
                        20  10  10  10  10  10  10  20  20  20  20  20  20
                          20  20  20  20  20  20  20  20  20  20  20  20  20
  end fill
' --- Fuel block arrays -----------------------------------------------------
  ara=241  nux=9  nuy=9  nuz=1  typ=hexagonal
  fill
      1116  1116  1116  1116  1116  1116  1116  1116  1116
        1116  1116  1116  1116  2413  2413  2413  1315  1116
          1116  1116  1116  2413  2413  2413  2413  2413  1116
            1116  1116  2413  2413  2413  2413  2413  2413  1116
              1116  1412  2413  2413  1114  2413  2413  2413  1116
                1116  2413  2413  2413  2413  2413  2413  1116  1116
                  1116  2413  2413  2413  2413  2413  1116  1116  1116
                    1116  2413  2413  2413  1412  1116  1116  1116  1116
                      1116  1116  1116  1116  1116  1116  1116  1116  1116
  end fill

end array

' -------------------------------------------------------------------------------
' --- Energy splitting ------------------------------------------------------
read energy
  2e7 1.01e6 0.625 1e-5
end energy

' -------------------------------------------------------------------------------
' --- Plot cros-section -----------------------------------------------------
read plot
ttl='z=25 cm'
  TYP=XY
  XUL=-205.0 YUL=205.0  ZUL=25.
  XLR=205.0  YLR=-205.0 ZLR=25.
  NAX=640 end
ttl='Vertical View of the HTTR Core'
  TYP=XZ
  XUL=-205. YUL=0.  ZUL=30.
  XLR=205.  YLR=0. ZLR=-30.
  UAX=1.0 WDN=-1.0 NAX=640 end
end plot

end data
end
' -------------------------------------------------------------------------------
' --- End input deck --------------------------------------------------------
```

APPENDIX E

SCHEMATIC DIAGRAMS OF THE HTTR BENCHMARK CASE

Presented here is a schematic diagram of the HTTR benchmark case (Test2r3_Mg).





APPENDIX F

IR F-FACTOR

Nuclides for which IR f-factors are applied

Am-241	Np-235	U-232
Am-242	Np-236	U-233
Am-242m	Np-237	U-234
Am-243	Np-238	U-235
Am-244	Np-239	U-236
Am-244m	Pa-231	U-237
Bk-249	Pa-232	U-238
Bk-250	Pa-233	U-239
Cf-249	Pu-236	U-240
Cf-250	Pu-237	U-241
Cf-251	Pu-238	
Cf-252	Pu-239	
Cf-253	Pu-240	
Cf-254	Pu-241	
Cm-241	Pu-242	
Cm-242	Pu-243	
Cm-243	Pu-244	
Cm-244	Pu-246	
Cm-245	Ra-223	
Cm-246	Ra-226	
Cm-247	Th-227	
Cm-248	Th-228	
Cm-249	Th-229	
Cm-250	Th-230	
Es-254	Th-232	
Es-255	Th-233	
Fm-255	Th-234	

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11. ABSTRACT *(200 words or less)*

With current and ongoing interest in high temperature gas reactors (HTGRs), the U. S. Nuclear Regulatory Commission (NRC) anticipates the need for nuclear data libraries appropriate for use in applications for modeling, assessing, and analyzing HTGR reactor physics and operating behavior. The objective of this work was to develop a broad-group library suitable for production analysis with SCALE for HTGR applications. Several interim libraries were generated from SCALE fine-group 238-group and 999-group libraries, and the final broad-group library was created from Evaluated Nuclear Data File/B Version and other codes. Furthermore, intermediate resonance (IR) methods were applied to the HTGR broad-group library, and lambda factors and f-factors were incorporated into the library's nuclear data files. A new version of the SCALE BONAMI module, named BONAMI-IR, was developed to process the IR data in the new library and, thus, eliminate the need for the CENTRM/PMC modules for resonance self-shielding. This report documents the development of the HTGR broad-group nuclear data library and the results of test and benchmark calculations using the new library with SCALE. The 81-group library is shown to model HTGR cases with similar accuracy to the SCALE 238-group library but with significantly faster computational times due to the reduced number of energy groups and the use of BONAMI-IR instead of BONAMI/CENTRM/PMC for resonance self-shielding calculations.

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